

Supplementary Table 5. Inhibitor screening of GEPNET cell lines.

| Product Name | CAS Number | Form | Targets | GOT1 | | BON-1 | | QGP-1 | | P-ST5 | |
|--|--------------|---------------|---------------------------|--------------|---------|--------------|---------|--------------|---------|--------------|---------|
| | | | | % of control | Z-score | % of control | Z-score | % of control | Z-score | % of control | Z-score |
| (-)-Blebbistatin | 856925-71-8 | free base | ATPase | 77.9 | -0.36 | 77.6 | -0.31 | | | 95.6 | 0.09 |
| (-)-MK 801 Maleate | 121917-57-5 | maleate | GluR | 93.9 | 0.32 | 114.8 | 1.05 | 97.5 | -0.04 | 77.1 | -0.50 |
| (-)-Parthenolide | 20554-84-1 | free base | E3 Ligase | 107.6 | 0.90 | 77.7 | -0.30 | 85.6 | -0.54 | 135.5 | 1.35 |
| (-)-p-Bromotetramisole Oxalate | 62284-79-1 | free base | Others | 85.7 | -0.03 | 97.3 | 0.41 | 110.1 | 0.49 | 113.0 | 0.64 |
| (+)-Bicuculline | 485-49-4 | free base | GABA Receptor | 85.1 | -0.05 | 99.2 | 0.48 | 76.5 | -0.93 | 120.0 | 0.86 |
| (+)-JQ1 | 1268524-70-4 | free base | Epigenetic Reader Domain | 13.8 | -3.08 | 35.4 | -1.84 | | | 3.8 | -2.82 |
| (+)-Matrine | 519-02-8 | free base | Opioid Receptor | 121.8 | 1.50 | 102.0 | 0.58 | 83.6 | -0.63 | 124.5 | 1.00 |
| (R)-Nepicastat HCl | 195881-94-8 | Salt | Hydroxylase | 87.9 | 0.06 | 65.7 | -0.74 | 81.7 | -0.71 | 127.5 | 1.10 |
| (S)-crizotinib | 1374356-45-2 | free base | MTH | 107.2 | 0.88 | 79.4 | -0.24 | 105.1 | 0.28 | 97.0 | 0.13 |
| 10058-F4 | 403811-55-2 | free base | c-Myc | 82.3 | -0.18 | 97.2 | 0.41 | | | 99.2 | 0.20 |
| 17-AAG (Tanespimycin) | 75747-14-7 | free base | HSP (e.g. HSP90) | 67.9 | -0.78 | 26.5 | -2.16 | 59.2 | -1.67 | 53.4 | -1.25 |
| 17-DMAG (Alvespimycin) HCl | 467214-21-7 | hydrochloride | HSP (e.g. HSP90) | 39.4 | -1.99 | 26.4 | -2.17 | 41.7 | -2.41 | 21.9 | -2.25 |
| 1-Azakenpauillone | 676596-65-9 | free base | GSK-3 | 64.5 | -0.93 | 55.0 | -1.13 | | | 113.8 | 0.66 |
| 2-Methoxyestradiol (2-MeOE2) | 362-07-2 | free base | HIF | 93.0 | 0.28 | 81.3 | -0.17 | 116.6 | 0.77 | 94.9 | 0.07 |
| 3-Aminobenzamide | 3544-24-9 | free base | PARP | 72.5 | -0.59 | 74.6 | -0.42 | 85.1 | -0.57 | 116.1 | 0.74 |
| 3-Deazaneplanocin A (DZNeP) | 102052-95-9 | free base | Histone Methyltransferase | 75.4 | -0.47 | 64.8 | -0.77 | | | 105.3 | 0.40 |
| 3-Methyladenine | 5142-23-4 | free base | Autophagy,PI3K | 114.2 | 1.18 | 64.4 | -0.79 | 105.3 | 0.29 | 109.4 | 0.52 |
| 4E1RCat | 328998-25-0 | free base | ELF4 | 134.8 | 2.05 | 109.3 | 0.85 | 111.9 | 0.57 | 87.9 | -0.15 |
| 4EGI-1 | 315706-13-9 | free base | ELF4 | 80.9 | -0.23 | 116.5 | 1.11 | 101.3 | 0.12 | 128.6 | 1.13 |
| 5-hydroxymethyl Tolterodine (PNU 200577, 5-HMT, 5-HM) | 207679-81-0 | free base | AChR | 120.1 | 1.43 | 79.3 | -0.24 | 111.2 | 0.54 | 87.2 | -0.18 |
| 6H05 | No | free base | Rho | 90.1 | 0.16 | 116.8 | 1.12 | 108.4 | 0.42 | 132.9 | 1.27 |
| A66 | 1166227-08-2 | free base | PI3K | 60.3 | -1.11 | 114.1 | 1.02 | 78.7 | -0.84 | 115.3 | 0.71 |
| A-674563 | 552325-73-2 | free base | PKA,CDK,Akt | 51.0 | -1.50 | 114.8 | 1.05 | 94.7 | -0.16 | 59.7 | -1.05 |
| A-769662 | 844499-71-4 | free base | AMPK | 103.3 | 0.71 | 101.6 | 0.57 | 118.9 | 0.87 | 121.1 | 0.90 |

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|-------------------------------------|--------------|---------------|-----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| A-803467 | 944261-79-4 | free base | Sodium Channel | 119.4 | 1.40 | 105.0 | 0.69 | 89.5 | -0.38 | 108.2 | 0.49 |
| A922500 | 959122-11-3 | free base | Transferase | 85.0 | -0.06 | 66.4 | -0.71 | 62.4 | -1.53 | 110.6 | 0.56 |
| ABT-199 (GDC-0199) | 1257044-40-8 | free base | Bcl-2 | 68.4 | -0.76 | 63.8 | -0.81 | 102.9 | 0.19 | 41.2 | -1.63 |
| ABT-263 (Navitoclax) | 923564-51-6 | free base | Bcl-2 | 123.3 | 1.56 | 114.4 | 1.03 | 86.1 | -0.52 | 4.2 | -2.81 |
| ABT-737 | 852808-04-9 | free base | Autophagy,Bcl-2 | 128.9 | 1.80 | 114.2 | 1.03 | 97.6 | -0.04 | 3.8 | -2.82 |
| AC480 (BMS-599626) | 714971-09-2 | free base | HER2,EGFR | 93.7 | 0.31 | 105.0 | 0.69 | 113.8 | 0.65 | 106.6 | 0.44 |
| Acadesine | 2627-69-2 | free base | AMPK | 101.8 | 0.65 | 113.6 | 1.01 | 102.0 | 0.15 | 93.1 | 0.01 |
| Acebutolol HCl | 34381-68-5 | hydrochloride | Adrenergic Receptor | 94.2 | 0.33 | 115.3 | 1.06 | 111.8 | 0.57 | 135.6 | 1.35 |
| Acemetacin | 53164-05-9 | free base | COX | 85.6 | -0.03 | 49.6 | -1.32 | 122.5 | 1.02 | 107.6 | 0.47 |
| Acetylcholine Chloride | 60-31-1 | chloride | AChR | 108.1 | 0.92 | 105.1 | 0.69 | 108.3 | 0.42 | 92.0 | -0.03 |
| Acetylcysteine | 616-91-1 | free base | AChR | 83.6 | -0.12 | 65.4 | -0.75 | 89.1 | -0.40 | 98.0 | 0.16 |
| Aclidinium Bromide | 320345-99-1 | free base | AChR | 96.8 | 0.44 | 112.5 | 0.96 | 100.9 | 0.10 | 128.7 | 1.14 |
| Adefovir Dipivoxil | 142340-99-6 | free base | Reverse Transcriptase | 115.8 | 1.25 | 99.8 | 0.50 | 98.8 | 0.02 | 28.4 | -2.04 |
| ADL5859 HCl | 850173-95-4 | hydrochloride | Opioid Receptor | 84.1 | -0.10 | 116.4 | 1.11 | 110.1 | 0.49 | 64.2 | -0.91 |
| Adrenalone HCl | 62-13-5 | hydrochloride | Adrenergic Receptor | 94.9 | 0.36 | 118.5 | 1.18 | 109.3 | 0.46 | 129.8 | 1.17 |
| ADX-47273 | 851881-60-2 | free base | GluR | 82.6 | -0.16 | 51.3 | -1.26 | 120.8 | 0.95 | 130.7 | 1.20 |
| AEBSF HCl | 30827-99-7 | Salt | Serine Protease | 92.6 | 0.26 | 57.3 | -1.04 | 102.4 | 0.17 | 112.3 | 0.62 |
| AEE788 (NVP-AEE788) | 497839-62-0 | free base | HER2,VEGFR,EGFR | 100.1 | 0.58 | 115.8 | 1.08 | 119.9 | 0.91 | 96.3 | 0.11 |
| Afatinib (BIBW2992) | 439081-18-2 | free base | EGFR,HER2 | 100.7 | 0.61 | 105.4 | 0.71 | 96.0 | -0.11 | 90.9 | -0.06 |
| AG-1024 | 65678-07-1 | free base | IGF-1R | 100.0 | 0.58 | 102.3 | 0.59 | 85.5 | -0.55 | 93.0 | 0.01 |
| AG-14361 | 328543-09-5 | free base | PARP | 106.4 | 0.85 | 55.0 | -1.13 | 96.1 | -0.10 | 77.9 | -0.47 |
| AG-1478 (Tyrphostin AG-1478) | 153436-53-4 | free base | EGFR | 99.2 | 0.54 | 105.6 | 0.71 | 119.4 | 0.89 | 123.9 | 0.99 |
| AG-18 | 118409-57-7 | free base | EGFR | 85.7 | -0.03 | 66.5 | -0.71 | 106.2 | 0.33 | 86.8 | -0.19 |
| AG-490 (Tyrphostin B42) | 133550-30-8 | free base | JAK,EGFR | 102.6 | 0.69 | 117.0 | 1.13 | 117.2 | 0.80 | 93.4 | 0.02 |
| AGI-5198 | 1355326-35-0 | free base | Dehydrogenase | 86.7 | 0.01 | 77.8 | -0.30 | | | 114.5 | 0.69 |
| AGI-6780 | 1432660-47-3 | free base | IDH2 | 70.6 | -0.67 | 107.4 | 0.78 | | | 102.6 | 0.31 |
| Agomelatine | 138112-76-2 | free base | 5-HT Receptor | 113.7 | 1.16 | 112.9 | 0.98 | 111.5 | 0.55 | 67.1 | -0.81 |
| Alfuzosin HCl | 81403-68-1 | hydrochloride | Adrenergic Receptor | 90.0 | 0.15 | 56.3 | -1.08 | 108.9 | 0.44 | 91.8 | -0.03 |
| Alisertib (MLN8237) | 1028486-01-2 | free base | Aurora Kinase | 91.9 | 0.23 | 73.8 | -0.44 | 71.1 | -1.16 | 60.7 | -1.02 |

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|-------------------------------|-------------|-----------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Aliskiren Hemifumarate | 173334-58-2 | fumarate | RAAS | 87.6 | 0.05 | 66.7 | -0.70 | 91.6 | -0.29 | 124.8 | 1.01 |
| Alizarin | 72-48-0 | free base | P450 (e.g. CYP17) | 94.8 | 0.36 | 51.8 | -1.25 | 118.4 | 0.85 | 123.8 | 0.98 |
| Allopurinol | 315-30-0 | free base | OX Receptor | 107.6 | 0.90 | 114.9 | 1.05 | 110.5 | 0.51 | 94.8 | 0.06 |
| Almorexant HCl | 913358-93-7 | HCl | OX Receptor | 114.8 | 1.20 | 67.7 | -0.67 | 106.7 | 0.35 | 100.2 | 0.23 |
| Almotriptan Malate | 181183-52-8 | malate | 5-HT Receptor | 134.3 | 2.03 | 114.4 | 1.03 | 97.0 | -0.06 | 92.4 | -0.01 |
| Alogliptin | 850649-61-5 | free base | DPP-4 | 83.7 | -0.12 | 68.0 | -0.65 | 128.1 | 1.26 | 103.6 | 0.34 |
| Aloxistatin | 88321-09-9 | free base | Cysteine protease | 72.4 | -0.59 | 117.1 | 1.13 | 99.5 | 0.04 | 69.1 | -0.75 |
| Altrenogest | 850-52-2 | free base | Estrogen/progestogen Receptor | 93.6 | 0.30 | 114.7 | 1.04 | 115.4 | 0.72 | 125.6 | 1.04 |
| Alvelestat (AZD9668) | 848141-11-7 | free base | Serine Protease | 77.8 | -0.36 | 79.4 | -0.24 | | | 133.0 | 1.27 |
| AM1241 | 444912-48-5 | free base | Cannabinoid Receptor | 101.5 | 0.64 | 114.8 | 1.05 | 110.4 | 0.51 | 84.0 | -0.28 |
| AM251 | 183232-66-8 | free base | Cannabinoid Receptor | 89.7 | 0.14 | 92.4 | 0.23 | 108.3 | 0.42 | 116.8 | 0.76 |
| Amantadine HCl | 665-66-7 | hydrochloride | Dopamine Receptor | 111.7 | 1.07 | 108.8 | 0.83 | 98.7 | 0.01 | 115.9 | 0.73 |
| Ambroxol HCl | 23828-92-4 | hydrochloride | Sodium Channel | 89.6 | 0.14 | 93.1 | 0.26 | 87.3 | -0.47 | 117.7 | 0.79 |
| Amfebutamone HCl | 31677-93-7 | hydrochloride | Dopamine Receptor, AChR | 105.8 | 0.82 | 109.7 | 0.86 | 138.5 | 1.70 | 111.9 | 0.60 |
| AMG-458 | 913376-83-7 | free base | c-Met | 74.7 | -0.49 | 77.0 | -0.33 | 86.1 | -0.52 | 111.7 | 0.60 |
| AMG-517 | 659730-32-2 | free base | TRPV | 80.7 | -0.24 | 93.4 | 0.27 | | | 120.2 | 0.87 |
| AMG-900 | 945595-80-2 | free base | Aurora Kinase | 74.8 | -0.49 | 51.5 | -1.25 | 68.3 | -1.28 | 90.4 | -0.08 |
| Aminoglutethimide | 125-84-8 | free base | Aromatase | 129.1 | 1.81 | 99.9 | 0.50 | 104.4 | 0.25 | 72.7 | -0.64 |
| Aminophylline | 317-34-0 | ethylenediamine | PDE | 84.7 | -0.07 | 112.8 | 0.97 | 100.6 | 0.09 | 93.6 | 0.03 |
| Amiodarone HCl | 19774-82-4 | hydrochloride | Autophagy, Potassium Channel | 89.3 | 0.12 | 114.9 | 1.05 | 101.5 | 0.13 | 80.2 | -0.40 |
| Amisulpride | 71675-85-9 | free base | Dopamine Receptor | 70.3 | -0.68 | 82.2 | -0.14 | 137.7 | 1.67 | 94.3 | 0.05 |
| Amitriptyline HCl | 549-18-8 | hydrochloride | 5-HT Receptor | 90.9 | 0.19 | 118.0 | 1.16 | 106.2 | 0.33 | 138.2 | 1.44 |
| Amlodipine | 88150-42-9 | free base | Calcium Channel | 91.6 | 0.22 | 116.6 | 1.11 | 103.6 | 0.22 | 156.6 | 2.02 |
| Amonafide | 69408-81-7 | free base | Topoisomerase | 69.9 | -0.70 | 113.6 | 1.00 | 78.4 | -0.85 | 81.4 | -0.36 |
| Ampiroxicam | 99464-64-9 | free base | COX | 99.2 | 0.54 | 118.0 | 1.16 | 112.5 | 0.60 | 128.5 | 1.13 |
| Amprenavir | 161814-49-9 | free base | HIV Protease | 88.1 | 0.07 | 113.3 | 0.99 | 109.6 | 0.47 | 91.3 | -0.05 |
| Amuvatinib (MP-470) | 850879-09-3 | free base | FLT3,c-RET,PDGFR,c-Kit | 97.7 | 0.48 | 81.8 | -0.15 | 122.3 | 1.01 | 58.0 | -1.10 |
| Anacetrapib (MK-0859) | 875446-37-0 | free base | CETP | 81.4 | -0.21 | 63.4 | -0.82 | 116.9 | 0.78 | 125.3 | 1.03 |

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|---------------------------------|--------------|---------------|--|-------|-------|-------|-------|-------|-------|-------|-------|
| Anagrelide HCl | 58579-51-4 | hydrochloride | PDE | 92.1 | 0.24 | 118.6 | 1.18 | 111.3 | 0.54 | 122.0 | 0.92 |
| Anastrozole | 120511-73-1 | free base | Aromatase | 83.7 | -0.11 | 112.4 | 0.96 | 113.0 | 0.62 | 77.6 | -0.48 |
| Andarine | 401900-40-1 | free base | Androgen Receptor | 101.7 | 0.65 | 117.3 | 1.14 | 115.2 | 0.71 | 57.1 | -1.13 |
| Anidulafungin (LY303366) | 166663-25-8 | free base | Others | 100.7 | 0.61 | 104.5 | 0.67 | 86.9 | -0.49 | 92.8 | 0.00 |
| Aniracetam | 72432-10-1 | free base | AMPA Receptor-kainate Receptor-NMDA Receptor | 96.8 | 0.44 | 73.1 | -0.47 | 119.5 | 0.89 | 94.1 | 0.04 |
| AP26113 | 1197958-12-5 | free base | ALK | 54.9 | -1.33 | 60.9 | -0.91 | 64.6 | -1.44 | 108.9 | 0.51 |
| Apatinib | 811803-05-1 | sulfate | VEGFR | 113.1 | 1.13 | 113.6 | 1.00 | 100.1 | 0.07 | 92.9 | 0.00 |
| Apigenin | 520-36-5 | free base | P450 (e.g. CYP17) | 108.5 | 0.93 | 107.3 | 0.77 | 82.6 | -0.67 | 119.0 | 0.83 |
| Apixaban | 503612-47-3 | free base | Factor Xa | 89.2 | 0.12 | 114.8 | 1.05 | 90.2 | -0.35 | 90.7 | -0.07 |
| Apoptosis Activator 2 | 79183-19-0 | free base | Caspase | 78.8 | -0.32 | 64.9 | -0.77 | 129.1 | 1.30 | 104.6 | 0.37 |
| Apremilast (CC-10004) | 608141-41-9 | free base | PDE | 89.2 | 0.12 | 64.5 | -0.78 | 112.1 | 0.58 | 96.1 | 0.10 |
| Aprepitant | 170729-80-3 | free base | Substance P | 90.6 | 0.18 | 104.5 | 0.67 | 117.4 | 0.80 | 71.9 | -0.66 |
| AR-42 | 935881-37-1 | free base | HDAC | 26.9 | -2.52 | 39.1 | -1.70 | 46.4 | -2.21 | 0.2 | -2.93 |
| AR-A014418 | 487021-52-3 | free base | GSK-3 | 78.5 | -0.33 | 116.7 | 1.12 | 129.3 | 1.31 | 73.5 | -0.61 |
| Arecoline | 300-08-3 | HBr | AChR | 85.8 | -0.03 | 56.3 | -1.08 | 104.0 | 0.24 | 125.4 | 1.03 |
| Aripiprazole | 129722-12-9 | free base | 5-HT Receptor | 95.9 | 0.40 | 106.4 | 0.74 | 100.5 | 0.08 | 155.0 | 1.97 |
| ARN-509 | 956104-40-8 | free base | Androgen Receptor | 88.3 | 0.08 | 77.1 | -0.32 | 111.6 | 0.56 | 108.5 | 0.50 |
| ARQ 621 | 1095253-39-6 | free base | Kinesin | 64.4 | -0.93 | 77.2 | -0.32 | 45.6 | -2.24 | 58.6 | -1.08 |
| AS-252424 | 900515-16-4 | free base | PI3K | 67.5 | -0.80 | 115.8 | 1.08 | 112.5 | 0.60 | 83.0 | -0.31 |
| AS-604850 | 648449-76-7 | free base | PI3K | 85.0 | -0.06 | 53.2 | -1.19 | 113.2 | 0.63 | 125.2 | 1.03 |
| Asaraldehyde | 4460-86-0 | free base | COX | 103.9 | 0.74 | 70.0 | -0.58 | 118.5 | 0.85 | 117.0 | 0.77 |
| Asenapine | 85650-56-2 | maleate | 5-HT Receptor,Adrenergic Receptor | 90.9 | 0.19 | 54.9 | -1.13 | 113.6 | 0.64 | 94.1 | 0.04 |
| Asiatic Acid | 464-92-6 | free base | p38 MAPK | 108.7 | 0.94 | 69.8 | -0.59 | 89.5 | -0.38 | 114.3 | 0.68 |
| Aspirin | 50-78-2 | free base | Proteasome | 151.0 | 2.74 | 111.9 | 0.94 | 109.7 | 0.48 | 93.3 | 0.02 |
| AST-1306 | 1050500-29-2 | mesylate | EGFR | 80.6 | -0.25 | 64.8 | -0.77 | 73.6 | -1.06 | 77.0 | -0.50 |
| Astragaloside A | 83207-58-3 | free base | TGF-beta/Smad | 104.7 | 0.77 | 102.9 | 0.61 | 82.9 | -0.66 | 114.7 | 0.69 |
| Astragaloside A | 83207-58-3 | free base | TGF-beta/Smad | 103.1 | 0.71 | 89.5 | 0.13 | 87.7 | -0.46 | 117.9 | 0.79 |
| AT101 | 866541-93-7 | free base | Bcl-2 | 75.5 | -0.46 | 113.6 | 1.00 | 118.6 | 0.85 | 112.1 | 0.61 |

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|---------------------------------|--------------|--------------------|---------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| AT13387 | 912999-49-6 | free base | HSP (e.g. HSP90) | 55.4 | -1.32 | 29.3 | -2.06 | 43.4 | -2.34 | 38.6 | -1.72 |
| AT7519 | 844442-38-2 | free base | CDK | 59.5 | -1.14 | 27.1 | -2.14 | 31.3 | -2.86 | 19.4 | -2.32 |
| AT7867 | 857531-00-1 | free base | S6 Kinase,Akt | 86.2 | -0.01 | 115.4 | 1.07 | 115.7 | 0.73 | 108.3 | 0.49 |
| AT9283 | 896466-04-9 | free base | JAK,Aurora Kinase,Bcr-Abl | 77.0 | -0.40 | 109.8 | 0.87 | 60.3 | -1.62 | 88.1 | -0.15 |
| Ataluren (PTC124) | 775304-57-9 | free base | CFTR | 88.0 | 0.07 | 56.5 | -1.07 | 82.4 | -0.68 | 112.9 | 0.64 |
| Atazanavir Sulfate | 229975-97-7 | sulfate | HIV Protease | 76.4 | -0.43 | 94.9 | 0.32 | 98.3 | -0.01 | 93.1 | 0.01 |
| Atglistatin | 1469924-27-3 | free base | ATGL | 85.8 | -0.03 | 64.5 | -0.78 | 109.1 | 0.45 | 108.7 | 0.50 |
| Atomoxetine HCl | 82248-59-7 | hydrochloride | 5-HT Receptor | 85.3 | -0.05 | 62.0 | -0.87 | 117.2 | 0.79 | 140.4 | 1.51 |
| Atorvastatin Calcium | 134523-03-8 | calcium | HMG-CoA Reductase | 92.2 | 0.24 | 107.5 | 0.78 | 95.1 | -0.14 | 111.2 | 0.58 |
| Atropine | 5908-99-6 | coordination co | AChR | 112.5 | 1.10 | 94.8 | 0.32 | 86.6 | -0.51 | 105.7 | 0.41 |
| Aurora A Inhibitor I | 1158838-45-9 | free base | Aurora Kinase | 50.6 | -1.52 | 46.7 | -1.43 | 62.9 | -1.51 | 59.3 | -1.06 |
| AUY922 (NVP-AUY922) | 747412-49-3 | free base | HSP (e.g. HSP90) | 40.6 | -1.94 | 36.3 | -1.81 | 34.5 | -2.72 | 47.8 | -1.43 |
| Avagacestat (BMS-708163) | 1146699-66-2 | free base | Gamma-secretase,Beta Amyloid | 130.5 | 1.87 | 91.9 | 0.21 | 110.4 | 0.51 | 93.9 | 0.03 |
| Avanafil | 330784-47-9 | free base | PDE | 90.2 | 0.16 | 53.5 | -1.18 | 104.3 | 0.25 | 125.9 | 1.05 |
| Avasimibe | 166518-60-1 | free base | P450 (e.g. CYP17) | 104.1 | 0.75 | 69.0 | -0.62 | 94.4 | -0.17 | 81.2 | -0.37 |
| AVL-292 | 1202757-89-8 | free base | BTK | 76.1 | -0.43 | 81.3 | -0.17 | | | 92.1 | -0.02 |
| Axitinib | 319460-85-0 | free base | c-Kit,VEGFR,PDGFR | 121.5 | 1.49 | 114.8 | 1.05 | 80.9 | -0.75 | 96.1 | 0.10 |
| AZ 3146 | 1124329-14-1 | free base | Kinesin | 69.2 | -0.73 | 90.1 | 0.15 | 139.0 | 1.72 | 132.3 | 1.25 |
| AZ 628 | 878739-06-1 | free base | Raf | 72.3 | -0.60 | 37.8 | -1.75 | 56.6 | -1.78 | 104.0 | 0.35 |
| AZ 960 | 905586-69-8 | free base | JAK | 61.7 | -1.05 | 66.5 | -0.71 | 42.6 | -2.37 | 79.8 | -0.41 |
| AZ20 | 1233339-22-4 | free base | ATM/ATR | 57.6 | -1.22 | 46.2 | -1.45 | 80.3 | -0.77 | 58.4 | -1.09 |
| Azacitidine | 320-67-2 | free base | DNA Methyltransferase | 117.9 | 1.33 | 115.6 | 1.08 | 117.0 | 0.79 | 80.7 | -0.38 |
| Azatadine dimaleate | 3978-86-7 | maleate | Histamine Receptor | 96.0 | 0.40 | 81.6 | -0.16 | 111.0 | 0.53 | 123.3 | 0.96 |
| AZD1080 | 612487-72-6 | free base | GSK-3 | 77.0 | -0.40 | 67.0 | -0.69 | | | 104.9 | 0.38 |
| AZD1208 | 1204144-28-4 | free base | Pim | 55.7 | -1.30 | 79.5 | -0.24 | | | 45.3 | -1.51 |
| AZD1480 | 935666-88-9 | free base | JAK | 80.1 | -0.27 | 103.2 | 0.63 | 77.2 | -0.90 | 74.1 | -0.59 |
| AZD1981 | 802904-66-1 | free base | GPR | 117.7 | 1.32 | 113.7 | 1.01 | 102.2 | 0.16 | 115.5 | 0.72 |
| AZD2014 | 1009298-59-2 | free base | mTOR | 57.7 | -1.21 | 60.5 | -0.93 | 71.9 | -1.13 | 61.8 | -0.98 |

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|--|--------------|---------------|------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| AZD2461 | 1174043-16-3 | free base | PARP | 78.0 | -0.36 | 72.6 | -0.49 | 82.7 | -0.67 | 120.3 | 0.87 |
| AZD2461 | 1174043-16-3 | free base | PARP | 85.8 | -0.03 | 58.4 | -1.00 | 77.3 | -0.90 | 121.2 | 0.90 |
| AZD2858 | 486424-20-8 | free base | GSK-3 | 74.5 | -0.50 | 104.8 | 0.68 | | | 70.6 | -0.70 |
| AZD3463 | 1356962-20-3 | free base | ALK | 30.8 | -2.36 | 69.0 | -0.62 | | | 69.6 | -0.74 |
| AZD3514 | 1240299-33-5 | free base | Androgen Receptor | 80.3 | -0.26 | 107.6 | 0.79 | 77.7 | -0.88 | 94.7 | 0.06 |
| AZD3514 | 1240299-33-5 | free base | Androgen Receptor | 81.4 | -0.21 | 79.2 | -0.25 | 79.8 | -0.79 | 114.9 | 0.70 |
| AZD4547 | 1035270-39-3 | free base | FGFR | 87.9 | 0.06 | 114.1 | 1.02 | 98.4 | 0.00 | 117.5 | 0.78 |
| AZD5363 | 1143532-39-1 | free base | Akt | 48.2 | -1.62 | 80.8 | -0.19 | 109.7 | 0.48 | 128.7 | 1.14 |
| AZD5438 | 602306-29-6 | free base | CDK | 69.5 | -0.71 | 51.8 | -1.25 | 99.0 | 0.02 | 86.4 | -0.20 |
| AZD6482 | 1173900-33-8 | free base | PI3K | 71.5 | -0.63 | 115.6 | 1.08 | 98.1 | -0.01 | 93.7 | 0.03 |
| AZD7545 | 252017-04-2 | free base | PDHK | 78.8 | -0.32 | 99.8 | 0.50 | 103.6 | 0.22 | 109.3 | 0.52 |
| AZD7762 | 860352-01-8 | free base | Chk | 46.6 | -1.69 | 13.7 | -2.63 | 112.7 | 0.60 | 19.6 | -2.32 |
| AZD8055 | 1009298-09-2 | free base | mTOR | 49.7 | -1.56 | 50.9 | -1.28 | 46.1 | -2.22 | 40.6 | -1.65 |
| AZD8330 | 869357-68-6 | free base | MEK | 100.9 | 0.61 | 23.9 | -2.26 | 42.5 | -2.38 | 102.7 | 0.31 |
| AZD8931 (Sapitinib) | 848942-61-0 | free base | HER2,EGFR | 109.5 | 0.98 | 60.2 | -0.94 | 75.4 | -0.98 | 79.9 | -0.41 |
| AZD9291 | 1421373-65-0 | free base | EGFR | 90.8 | 0.19 | 92.4 | 0.23 | 96.9 | -0.06 | 47.9 | -1.42 |
| Azelastine HCl | 79307-93-0 | hydrochloride | Histamine Receptor | 110.0 | 1.00 | 111.0 | 0.91 | 124.1 | 1.09 | 131.4 | 1.22 |
| Azelnidipine | 123524-52-7 | free base | Calcium Channel | 75.7 | -0.45 | 73.9 | -0.44 | 109.3 | 0.46 | 120.5 | 0.88 |
| Azilsartan | 147403-03-0 | free base | RAAS | 90.8 | 0.19 | 55.9 | -1.09 | 116.4 | 0.76 | 112.9 | 0.64 |
| Azilsartan Medoxomil | 863031-21-4 | free base | RAAS | 92.6 | 0.26 | 119.9 | 1.23 | 109.9 | 0.49 | 124.7 | 1.01 |
| Azithromycin | 83905-01-5 | free base | Autophagy | 83.5 | -0.12 | 108.8 | 0.83 | 114.2 | 0.67 | 81.8 | -0.35 |
| Baicalein | 491-67-8 | free base | P450 (e.g. CYP17) | 84.5 | -0.08 | 60.3 | -0.94 | 89.2 | -0.39 | 117.5 | 0.78 |
| Bambuterol HCl | 81732-46-9 | Salt | Adrenergic Receptor | 87.7 | 0.05 | 61.1 | -0.91 | 82.3 | -0.69 | 127.7 | 1.11 |
| BAPTA-AM | 126150-97-8 | free base | Others | 68.3 | -0.77 | 70.1 | -0.58 | 94.8 | -0.16 | 95.6 | 0.09 |
| Barasertib (AZD1152-HQPA) | 722544-51-6 | free base | Aurora Kinase | 90.6 | 0.18 | 82.0 | -0.14 | 74.4 | -1.02 | 62.1 | -0.97 |
| Bardoxolone Methyl | 218600-53-4 | free base | IκB/IKK | 45.1 | -1.75 | 31.2 | -1.99 | 78.1 | -0.86 | 57.1 | -1.13 |
| Baricitinib (LY3009104, INCB028050) | 1187594-09-7 | free base | JAK | 71.6 | -0.63 | 94.9 | 0.33 | 125.6 | 1.15 | 102.8 | 0.32 |
| Batimastat (BB-94) | 130370-60-4 | free base | MMP | 71.7 | -0.62 | 67.9 | -0.66 | | | 106.4 | 0.43 |
| BAY 11-7082 | 19542-67-7 | free base | IκB/IKK,E2 conjugating | 76.0 | -0.44 | 57.1 | -1.05 | 117.6 | 0.81 | 94.0 | 0.04 |

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|--|--------------|---------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Bazedoxifene HCl | 198480-56-7 | free base | Estrogen/progestogen Receptor | 119.9 | 1.42 | 99.9 | 0.50 | 102.9 | 0.19 | 80.0 | -0.40 |
| Belinostat (PXD101) | 414864-00-9 | free base | HDAC | 35.8 | -2.14 | 67.9 | -0.66 | 63.3 | -1.49 | 2.1 | -2.87 |
| Benazepril HCl | 86541-74-4 | hydrochloride | RAAS | 88.1 | 0.07 | 82.2 | -0.14 | 109.8 | 0.48 | 91.3 | -0.05 |
| Benidipine HCl | 91599-74-5 | hydrochloride | Calcium Channel | 86.6 | 0.01 | 91.9 | 0.22 | 87.6 | -0.46 | 97.6 | 0.15 |
| Benserazide HCl | 14919-77-8 | hydrochloride | Dopamine Receptor,Others | 113.2 | 1.14 | 66.7 | -0.70 | 127.8 | 1.25 | 107.6 | 0.47 |
| Benzotropine mesylate | 132-17-2 | mesylate | Histamine Receptor | 97.4 | 0.47 | 117.4 | 1.14 | 110.9 | 0.53 | 124.3 | 1.00 |
| Bepotastine Besilate | 190786-44-8 | besilate | Histamine Receptor | 79.9 | -0.27 | 78.5 | -0.27 | 107.8 | 0.40 | 120.9 | 0.89 |
| Betahistine 2HCl | 5579-84-0 | 2HCl | Histamine Receptor | 91.9 | 0.23 | 117.5 | 1.14 | 116.5 | 0.77 | 145.1 | 1.66 |
| Beta-Lapachone | 4707-32-8 | free base | Topoisomerase | 91.4 | 0.21 | 103.0 | 0.62 | | | 86.3 | -0.21 |
| Betaxolol | 659-18-7 | free base | Adrenergic Receptor | 99.4 | 0.55 | 115.9 | 1.09 | 95.2 | -0.14 | 149.9 | 1.81 |
| Bethanechol chloride | 590-63-6 | chloride | AChR | 106.0 | 0.83 | 112.3 | 0.96 | 119.0 | 0.87 | 117.1 | 0.77 |
| Betulinic acid | 472-15-1 | free base | Topoisomerase | 95.2 | 0.37 | 116.2 | 1.10 | 114.4 | 0.68 | 95.0 | 0.07 |
| BGT226 (NVP-BGT226) | 1245537-68-1 | free base | PI3K,mTOR | 16.1 | -2.98 | 14.1 | -2.61 | 36.0 | -2.65 | -1.1 | -2.97 |
| BI 2536 | 755038-02-9 | free base | PLK | 40.8 | -1.93 | 39.2 | -1.70 | 43.0 | -2.36 | 4.4 | -2.80 |
| BIBR 1532 | 321674-73-1 | free base | Telomerase | 102.3 | 0.67 | 116.5 | 1.11 | 121.2 | 0.97 | 62.0 | -0.98 |
| Bicalutamide | 90357-06-5 | free base | Androgen Receptor | 105.7 | 0.82 | 107.2 | 0.77 | 135.0 | 1.55 | 75.0 | -0.57 |
| BI-D1870 | 501437-28-1 | free base | S6 Kinase | 83.2 | -0.13 | 82.3 | -0.14 | 105.2 | 0.29 | 73.4 | -0.61 |
| BIIB021 | 848695-25-0 | free base | HSP (e.g. HSP90) | 52.1 | -1.45 | 38.7 | -1.72 | 66.7 | -1.35 | 27.4 | -2.07 |
| BIO | 667463-62-9 | free base | GSK-3 | 61.8 | -1.04 | 91.4 | 0.19 | | | 132.2 | 1.25 |
| Biperiden HCl | 1235-82-1 | hydrochloride | AChR | 106.7 | 0.86 | 115.0 | 1.05 | 119.5 | 0.90 | 95.3 | 0.08 |
| BIRB 796 (Doramapimod) | 285983-48-4 | free base | p38 MAPK | 96.0 | 0.41 | 115.6 | 1.08 | 87.9 | -0.45 | 65.2 | -0.88 |
| Birinapant | 1260251-31-7 | free base | IAP | 85.4 | -0.04 | 92.5 | 0.24 | 82.3 | -0.68 | 127.3 | 1.09 |
| Bisoprolol fumarate | 104344-23-2 | free base | Adrenergic Receptor | 106.6 | 0.85 | 85.8 | -0.01 | 112.7 | 0.61 | 100.8 | 0.25 |
| BIX 01294 | 1392399-03-9 | hydrochloride | Histone Methyltransferase | 71.2 | -0.65 | 62.8 | -0.84 | 103.0 | 0.19 | 100.3 | 0.24 |
| BIX 02188 | 1094614-84-2 | free base | MEK | 84.0 | -0.10 | 115.8 | 1.08 | 114.4 | 0.68 | 95.2 | 0.08 |
| BIX 02189 | 1094614-85-3 | free base | MEK | 84.5 | -0.08 | 116.2 | 1.10 | 111.1 | 0.54 | 96.3 | 0.11 |
| BKM120 (NVP-BKM120, Buparlisib) | 944396-07-0 | free base | PI3K | 75.8 | -0.45 | 98.2 | 0.44 | 76.4 | -0.94 | 63.3 | -0.93 |
| BML-190 | 2854-32-2 | free base | Cannabinoid Receptor | 91.3 | 0.21 | 93.1 | 0.26 | 110.2 | 0.50 | 114.1 | 0.68 |

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|---|--------------|-----------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| BMN 673 | 1207456-01-6 | free base | PARP | 60.2 | -1.11 | 106.1 | 0.73 | 86.5 | -0.51 | 33.8 | -1.87 |
| BMS-265246 | 582315-72-8 | free base | CDK | 81.4 | -0.21 | 110.6 | 0.90 | 86.5 | -0.51 | 87.1 | -0.18 |
| BMS-345541 | 445430-58-0 | free base | IκB/IKK | 88.7 | 0.10 | 77.7 | -0.30 | 109.4 | 0.47 | 124.7 | 1.01 |
| BMS-378806 | 357263-13-9 | free base | gp120/CD4 | 98.0 | 0.49 | 111.9 | 0.94 | 108.8 | 0.44 | 123.7 | 0.98 |
| BMS-536924 | 468740-43-4 | free base | IGF-1R | 33.2 | -2.25 | 80.2 | -0.21 | 53.2 | -1.92 | 110.3 | 0.56 |
| BMS-707035 | 729607-74-3 | free base | Integrase | 51.9 | -1.46 | 46.2 | -1.45 | 63.4 | -1.49 | 29.1 | -2.02 |
| BMS-754807 | 1001350-96-4 | free base | IGF-1R,Trk receptor,c-Met | 28.2 | -2.47 | 49.9 | -1.31 | 45.8 | -2.24 | 55.0 | -1.20 |
| BMS-777607 | 1025720-94-8 | free base | Axl,c-Met | 104.9 | 0.79 | 115.3 | 1.06 | 112.9 | 0.61 | 78.5 | -0.45 |
| BMS-794833 | 1174046-72-0 | free base | VEGFR,c-Met | 100.8 | 0.61 | 50.5 | -1.29 | 138.8 | 1.71 | 98.9 | 0.19 |
| BMS-833923 | 1059734-66-5 | free base | Hedgehog/Smoothened | 74.8 | -0.49 | 93.8 | 0.28 | | | 117.3 | 0.78 |
| BMV 7378 | 21102-95-4 | dihydrochloride | 5-HT Receptor | 69.5 | -0.72 | 91.2 | 0.19 | 137.7 | 1.67 | 91.8 | -0.03 |
| Bortezomib (PS-341) | 179324-69-7 | free base | Proteasome | 5.2 | -3.44 | 2.4 | -3.04 | 27.5 | -3.01 | 3.6 | -2.83 |
| Bosentan | 147536-97-8 | free base | Endothelin Receptor | 84.3 | -0.09 | 71.7 | -0.52 | 78.6 | -0.84 | 129.2 | 1.15 |
| Bosentan Hydrate | 157212-55-0 | hydrate | Endothelin Receptor | 98.0 | 0.49 | 78.5 | -0.27 | 112.7 | 0.60 | 128.8 | 1.14 |
| Bosutinib (SKI-606) | 380843-75-4 | free base | Src | 80.9 | -0.23 | 94.6 | 0.31 | 142.3 | 1.86 | 127.3 | 1.09 |
| Brefeldin A | 20350-15-6 | free base | ATPase,Autophagy | 1.9 | -3.58 | 1.7 | -3.06 | 23.2 | -3.20 | 2.1 | -2.87 |
| Brinzolamide | 138890-62-7 | free base | Carbonic Anhydrase | 89.9 | 0.15 | 63.6 | -0.81 | 109.7 | 0.48 | 142.7 | 1.58 |
| Brivanim (BMS-540215) | 649735-46-6 | free base | FGFR,VEGFR | 94.4 | 0.34 | 76.5 | -0.34 | 78.5 | -0.85 | 116.5 | 0.75 |
| Brivanim Alaninate (BMS-582664) | 649735-63-7 | alaninate | VEGFR,FGFR | 97.0 | 0.45 | 88.2 | 0.08 | 92.7 | -0.25 | 74.5 | -0.58 |
| BRL-15572 | 193611-72-2 | dihydrochloride | 5-HT Receptor | 120.0 | 1.42 | 73.0 | -0.47 | 123.6 | 1.07 | 113.9 | 0.67 |
| BRL-54443 | 57477-39-1 | free base | 5-HT Receptor | 102.2 | 0.67 | 93.3 | 0.27 | 127.7 | 1.24 | 84.6 | -0.26 |
| Bromosporine | N/A | free base | Epigenetic Reader Domain | 49.5 | -1.56 | 69.9 | -0.59 | | | 62.4 | -0.96 |
| Brompheniramine hydrogen maleate | 980-71-2 | maleate | Histamine Receptor | 81.8 | -0.20 | 56.1 | -1.09 | 123.2 | 1.05 | 91.0 | -0.06 |
| BS-181 HCl | 1397219-81-6 | hydrochloride | CDK | 99.9 | 0.57 | 47.1 | -1.42 | 106.1 | 0.33 | 93.2 | 0.01 |
| BTB06584 | 219793-45-0 | free base | Fo-ATPase | 131.0 | 1.89 | 109.3 | 0.85 | 98.8 | 0.01 | 130.4 | 1.19 |
| Bufexamac | 2438-72-4 | free base | COX | 96.0 | 0.41 | 88.1 | 0.08 | 111.0 | 0.53 | 131.1 | 1.21 |
| Bupivacaine HCl | 18010-40-7 | hydrochloride | cAMP | 118.6 | 1.36 | 82.2 | -0.14 | 120.6 | 0.94 | 113.5 | 0.65 |
| Butein | 487-52-5 | free base | EGFR | 78.9 | -0.32 | 75.3 | -0.39 | 85.3 | -0.56 | 139.8 | 1.49 |

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| BV-6 | 1001600-56-1 | free base | IAP | 62.1 | -1.03 | 83.0 | -0.11 | 105.3 | 0.29 | 113.0 | 0.64 |
| BX-795 | 702675-74-9 | free base | IκB/IKK,PDK-1 | 69.6 | -0.71 | 68.6 | -0.63 | 117.0 | 0.79 | 65.8 | -0.86 |
| BX-912 | 702674-56-4 | free base | PDK-1 | 93.0 | 0.28 | 84.5 | -0.06 | 93.2 | -0.22 | 54.0 | -1.23 |
| BYL719 | 1217486-61-7 | free base | PI3K | 54.1 | -1.37 | 111.9 | 0.94 | 85.0 | -0.57 | 107.0 | 0.45 |
| C646 | 328968-36-1 | free base | Histone Acetyltransferase | 75.3 | -0.47 | 90.8 | 0.17 | | | 125.5 | 1.04 |
| Cabozantinib (XL184, BMS-907351) | 849217-68-1 | free base | FLT3,Tie-2,c-Kit,c-Met,VEGFR,Axl | 123.9 | 1.59 | 109.6 | 0.86 | 132.4 | 1.44 | 89.1 | -0.12 |
| Cabozantinib malate (XL184) | 1140909-48-3 | Malate | VEGFR | 74.8 | -0.49 | 118.5 | 1.18 | 104.0 | 0.23 | 118.6 | 0.82 |
| Caffeic Acid Phenethyl Ester | 104594-70-9 | free base | NF-κB | 82.2 | -0.18 | 116.4 | 1.11 | 102.0 | 0.15 | 55.3 | -1.19 |
| CAL-101 (Idelalisib, GS-1101) | 870281-82-6 | free base | PI3K | 82.1 | -0.18 | 75.2 | -0.39 | 74.7 | -1.01 | 112.4 | 0.62 |
| Camptothecin | 7689-03-4 | free base | Topoisomerase | 30.7 | -2.36 | 14.5 | -2.60 | 96.3 | -0.09 | 3.4 | -2.83 |
| Canagliflozin | 842133-18-0 | free base | SGLT | 88.8 | 0.10 | 51.4 | -1.26 | 110.2 | 0.50 | 123.4 | 0.97 |
| Candesartan | 139481-59-7 | free base | RAAS | 90.9 | 0.19 | 114.7 | 1.04 | 111.0 | 0.53 | 90.2 | -0.08 |
| Candesartan Cilexetil | 145040-37-5 | free base | RAAS | 121.6 | 1.49 | 93.2 | 0.26 | 111.4 | 0.55 | 111.8 | 0.60 |
| Captopril | 62571-86-2 | free base | RAAS | 118.3 | 1.35 | 114.4 | 1.03 | 110.2 | 0.50 | 122.2 | 0.93 |
| Carbamazepine | 298-46-4 | free base | Autophagy,Sodium Channel | 117.8 | 1.33 | 113.9 | 1.01 | 104.2 | 0.25 | 93.1 | 0.01 |
| Carfilzomib (PR-171) | 868540-17-4 | free base | Proteasome | 22.9 | -2.69 | 1.7 | -3.06 | 23.2 | -3.20 | 2.2 | -2.87 |
| Carteolol HCl | 51781-21-6 | Salt | Adrenergic Receptor | 75.0 | -0.48 | 113.1 | 0.99 | 81.7 | -0.71 | 93.0 | 0.00 |
| Carvedilol | 72956-09-3 | free base | Adrenergic Receptor | 129.3 | 1.82 | 112.9 | 0.98 | 109.1 | 0.45 | 105.3 | 0.40 |
| CAY10505 | 1218777-13-9 | free base | PI3K | 76.2 | -0.43 | 57.6 | -1.03 | 110.6 | 0.51 | 123.2 | 0.96 |
| CCT128930 | 885499-61-6 | free base | Akt | 87.3 | 0.04 | 64.5 | -0.78 | 94.3 | -0.18 | 89.9 | -0.09 |
| CCT129202 | 942947-93-5 | free base | Aurora Kinase | 57.2 | -1.24 | 57.1 | -1.05 | 86.4 | -0.51 | 59.3 | -1.06 |
| CCT137690 | 1095382-05-0 | free base | Aurora Kinase | 64.5 | -0.93 | 57.3 | -1.04 | 68.0 | -1.29 | 97.1 | 0.14 |
| Cediranib (AZD2171) | 288383-20-0 | free base | VEGFR | 93.5 | 0.30 | 115.8 | 1.08 | 103.2 | 0.20 | 109.2 | 0.52 |
| Celecoxib | 169590-42-5 | free base | COX | 106.7 | 0.86 | 79.4 | -0.24 | 103.3 | 0.21 | 83.1 | -0.31 |
| CEP-18770 (Delanzomib) | 847499-27-8 | free base | Proteasome | 3.5 | -3.51 | 3.4 | -3.00 | 33.6 | -2.75 | 1.3 | -2.90 |
| CEP-32496 | 1188910-76-0 | free base | CSF-1R,Raf | 81.7 | -0.20 | 57.8 | -1.02 | 85.4 | -0.56 | 67.8 | -0.79 |
| CEP-33779 | 1257704-57-6 | free base | JAK | 83.9 | -0.11 | 64.0 | -0.80 | 119.6 | 0.90 | 116.4 | 0.75 |
| Cetirizine DiHCl | 83881-52-1 | hydrochloride | Histamine Receptor | 91.2 | 0.20 | 54.9 | -1.13 | 153.2 | 2.33 | 95.7 | 0.09 |

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|---------------------------------|--------------|---------------|-------------------------------------|--------|-------|-------|-------|-------|-------|-------|-------|
| CFTRinh-172 | 307510-92-5 | free base | CFTR | 78.5 | -0.33 | 50.4 | -1.29 | | | 91.6 | -0.04 |
| CGI1746 | 910232-84-7 | free base | BTK | 77.1 | -0.39 | 82.6 | -0.12 | 107.5 | 0.38 | 107.6 | 0.47 |
| CGK 733 | 905973-89-9 | free base | ATM/ATR | 79.7 | -0.28 | 55.4 | -1.11 | | | 114.9 | 0.70 |
| CGP 57380 | 522629-08-9 | free base | MNK | 77.1 | -0.40 | 116.0 | 1.09 | 119.6 | 0.90 | 103.6 | 0.34 |
| CGS 21680 HCl | 124431-80-7 | hydrochloride | 5-alpha Reductase | 117.80 | 1.33 | 60.4 | -0.93 | 92.5 | -0.26 | 120.7 | 0.88 |
| CH5132799 | 1007207-67-1 | free base | mTOR,PI3K | 58.6 | -1.18 | 50.3 | -1.30 | 102.4 | 0.17 | 126.7 | 1.07 |
| CH5138303 | 959763-06-5 | free base | HSP (e.g. HSP90) | 42.2 | -1.87 | 33.9 | -1.89 | 48.0 | -2.15 | 55.9 | -1.17 |
| CHIR-124 | 405168-58-3 | free base | Chk | 53.0 | -1.42 | 30.2 | -2.03 | 144.9 | 1.97 | 53.2 | -1.25 |
| CHIR-99021 (CT99021) HCl | 252917-06-9 | hydrochloride | GSK-3 | 84.2 | -0.10 | 50.3 | -1.30 | 116.0 | 0.75 | 119.7 | 0.85 |
| Chloroambucil | 305-03-3 | free base | DNA/RNA Synthesis | 85.8 | -0.03 | 118.1 | 1.17 | 100.8 | 0.10 | 102.7 | 0.31 |
| Chlorpheniramine Maleate | 113-92-8 | maleate | Histamine Receptor | 105.1 | 0.79 | 117.5 | 1.14 | 112.5 | 0.60 | 94.2 | 0.04 |
| Chlorpromazine HCl | 69-09-0 | hydrochloride | Potassium Channel,Dopamine Receptor | 105.2 | 0.80 | 79.8 | -0.23 | 117.9 | 0.83 | 90.5 | -0.07 |
| Chlorprothixene | 113-59-7 | free base | Dopamine Receptor | 105.9 | 0.83 | 112.8 | 0.97 | 105.5 | 0.30 | 108.2 | 0.49 |
| Chrysophanic Acid | 481-74-3 | free base | mTOR,EGFR | 137.7 | 2.17 | 110.4 | 0.89 | 86.0 | -0.53 | 124.8 | 1.01 |
| CI994 (Tacedinaline) | 112522-64-2 | free base | HDAC | 83.1 | -0.14 | 111.9 | 0.94 | 145.7 | 2.01 | 136.8 | 1.39 |
| Ciclopirox ethanolamine | 41621-49-2 | ethanolamine | ATPase | 117.0 | 1.30 | 111.8 | 0.94 | 111.2 | 0.54 | 102.3 | 0.30 |
| Cilazapril Monohydrate | 92077-78-6 | monohydrate | RAAS | 95.3 | 0.38 | 115.8 | 1.08 | 82.2 | -0.69 | 93.1 | 0.01 |
| Cilengitide | 188968-51-6 | free base | Integrin | 85.7 | -0.03 | 70.4 | -0.57 | 60.7 | -1.60 | 103.8 | 0.35 |
| Cilnidipine | 132203-70-4 | free base | Calcium Channel | 114.2 | 1.18 | 76.6 | -0.34 | 118.8 | 0.87 | 69.4 | -0.74 |
| Cilomilast | 153259-65-5 | free base | PDE | 91.7 | 0.22 | 66.3 | -0.72 | 132.1 | 1.43 | 67.3 | -0.81 |
| Cilostazol | 73963-72-1 | free base | PDE | 74.2 | -0.52 | 60.4 | -0.93 | 117.4 | 0.80 | 93.2 | 0.01 |
| Cimetidine | 51481-61-9 | free base | Histamine Receptor | 94.4 | 0.34 | 107.3 | 0.77 | 123.3 | 1.06 | 121.0 | 0.89 |
| Cinacalcet HCl | 364782-34-3 | hydrochloride | CaSR | 102.0 | 0.66 | 77.5 | -0.31 | 108.7 | 0.43 | 85.6 | -0.23 |
| Ciprofibrate | 52214-84-3 | free base | PPAR | 125.4 | 1.65 | 90.1 | 0.15 | 112.5 | 0.60 | 111.7 | 0.60 |
| Ciproxifan | 184025-18-1 | maleate | Histamine Receptor | 91.6 | 0.22 | 46.8 | -1.43 | 128.1 | 1.26 | 109.5 | 0.53 |
| Cisatracurium Besylate | 96946-42-8 | besylate | Adrenergic Receptor | 124.9 | 1.63 | 106.8 | 0.76 | 83.7 | -0.63 | 108.1 | 0.48 |
| CK-636 | 442632-72-6 | free base | Arp2/3 | 98.1 | 0.49 | 116.9 | 1.12 | 100.8 | 0.10 | 83.5 | -0.30 |
| Clarithromycin | 81103-11-9 | free base | P450 (e.g. CYP17) | 101.7 | 0.65 | 55.7 | -1.10 | 115.2 | 0.71 | 123.6 | 0.98 |

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|---------------------------------|--------------|---------------|--------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Clemastine Fumarate | 14976-57-9 | free base | Histamine Receptor | 106.5 | 0.85 | 117.1 | 1.13 | 110.4 | 0.51 | 97.9 | 0.16 |
| Clevidipine Butyrate | 167221-71-8 | free base | Calcium Channel | 98.6 | 0.52 | 112.7 | 0.97 | 101.1 | 0.11 | 101.5 | 0.27 |
| Clinofibrate | 30299-08-2 | free base | RAAS | 100.8 | 0.61 | 113.9 | 1.01 | 126.6 | 1.20 | 110.3 | 0.56 |
| Clomifene citrate | 50-41-9 | citrate | Estrogen/progestogen Receptor | 75.6 | -0.46 | 51.1 | -1.27 | 137.2 | 1.65 | 128.3 | 1.12 |
| Clomipramine HCl | 17321-77-6 | hydrochloride | 5-HT Receptor | 95.8 | 0.40 | 49.6 | -1.32 | 109.6 | 0.47 | 123.3 | 0.96 |
| Clonidine HCl | 4205-91-8 | hydrochloride | Adrenergic Receptor, Autophagy | 109.7 | 0.99 | 109.0 | 0.83 | 121.3 | 0.97 | 115.8 | 0.73 |
| Clopidogrel | 120202-66-6 | sulfate | P2 Receptor | 98.9 | 0.53 | 60.2 | -0.94 | 150.6 | 2.21 | 77.5 | -0.48 |
| Clozapine | 5786-21-0 | free base | 5-HT Receptor | 108.6 | 0.94 | 66.8 | -0.70 | 123.4 | 1.06 | 96.4 | 0.11 |
| CNX-2006 | 1375465-09-0 | free base | EGFR | 72.9 | -0.57 | 76.0 | -0.37 | | | 120.9 | 0.89 |
| CNX-774 | 1202759-32-7 | free base | BTK | 85.1 | -0.05 | 85.1 | -0.03 | | | 108.5 | 0.50 |
| CO-1686 (AVL-301) | 1374640-70-6 | free base | EGFR | 64.0 | -0.95 | 116.4 | 1.10 | 96.5 | -0.08 | 76.4 | -0.52 |
| Cobicistat (GS-9350) | 1004316-88-4 | free base | P450 (e.g. CYP17) | 77.4 | -0.38 | 115.6 | 1.08 | 121.4 | 0.97 | 96.0 | 0.10 |
| CORM-3 | 475473-26-8 | free base | Others | 78.0 | -0.36 | 71.6 | -0.52 | 81.8 | -0.71 | 80.8 | -0.38 |
| Costunolide | 553-21-9 | free base | Telomerase | 75.1 | -0.48 | 115.0 | 1.05 | 128.1 | 1.26 | 106.6 | 0.44 |
| CP-673451 | 343787-29-1 | free base | PDGFR | 96.2 | 0.41 | 115.2 | 1.06 | 162.6 | 2.72 | 100.7 | 0.25 |
| CP-724714 | 537705-08-1 | free base | EGFR,HER2 | 97.6 | 0.48 | 106.1 | 0.73 | 116.6 | 0.77 | 87.0 | -0.18 |
| CP-91149 | 186392-40-5 | free base | Phosphorylase | 101.9 | 0.66 | 81.9 | -0.15 | 124.4 | 1.10 | 125.1 | 1.02 |
| CPI-203 | 1446144-04-2 | free base | Epigenetic Reader Domain | 26.6 | -2.53 | 48.8 | -1.35 | 61.2 | -1.58 | 5.5 | -2.77 |
| CPI-613 | 95809-78-2 | free base | Dehydrogenase | 105.5 | 0.81 | 65.8 | -0.73 | 115.6 | 0.73 | 112.3 | 0.62 |
| Crenolanib (CP-868596) | 670220-88-9 | free base | PDGFR | 66.1 | -0.86 | 48.4 | -1.37 | 163.6 | 2.77 | 137.3 | 1.41 |
| Crizotinib (PF-02341066) | 877399-52-5 | free base | c-Met,ALK | 58.4 | -1.19 | 95.6 | 0.35 | 102.7 | 0.18 | 84.3 | -0.27 |
| CRT0044876 | 6960-45-8 | free base | APE | 81.8 | -0.20 | 104.0 | 0.66 | 78.0 | -0.87 | 69.2 | -0.75 |
| Cryptotanshinone | 35825-57-1 | free base | STAT | 106.1 | 0.83 | 49.5 | -1.33 | 97.5 | -0.04 | 91.1 | -0.05 |
| CTEP (RO4956371) | 871362-31-1 | free base | GluR | 96.8 | 0.44 | 114.7 | 1.04 | 114.5 | 0.68 | 116.7 | 0.76 |
| CUDC-101 | 1012054-59-9 | free base | HDAC,HER2,EGFR | 7.9 | -3.33 | 48.6 | -1.36 | 36.2 | -2.64 | 0.3 | -2.93 |
| CUDC-907 | 1339928-25-4 | free base | PI3K,HDAC | 73.1 | -0.57 | 114.9 | 1.05 | 104.6 | 0.26 | 94.7 | 0.06 |
| CW069 | | free base | Microtubule Associat | 76.9 | -0.40 | 116.1 | 1.10 | 95.5 | -0.12 | 75.2 | -0.56 |
| CX-6258 HCl | 1353859-00-3 | Salt | Pim | 58.2 | -1.20 | 75.4 | -0.39 | 66.6 | -1.35 | 11.4 | -2.58 |

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|---|--------------|---------------|----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| CX-6258 HCl | 1353859-00-3 | Salt | Pim | 64.7 | -0.92 | 106.5 | 0.75 | 68.6 | -1.27 | 26.4 | -2.11 |
| CYC116 | 693228-63-6 | free base | Aurora Kinase,VEGFR | 98.4 | 0.51 | 81.1 | -0.18 | 92.2 | -0.27 | 86.0 | -0.22 |
| Cyclizine 2HCl | 5897-18-7 | hydrochloride | Histamine Receptor | 132.2 | 1.94 | 118.5 | 1.18 | 95.6 | -0.12 | 124.5 | 1.00 |
| Cyclobenzaprine HCl | 6202-23-9 | Salt | Others | 77.0 | -0.40 | 117.4 | 1.14 | 81.2 | -0.73 | 101.8 | 0.28 |
| Cyproheptadine HCl | 969-33-5 | hydrochloride | Histamine Receptor | 100.1 | 0.58 | 110.7 | 0.90 | 97.3 | -0.05 | 122.7 | 0.95 |
| Cyproterone Acetate | 427-51-0 | acetate | Androgen Receptor | 103.4 | 0.72 | 115.8 | 1.08 | 106.2 | 0.33 | 94.6 | 0.06 |
| CYT387 | 1056634-68-4 | free base | JAK | 90.3 | 0.17 | 57.8 | -1.03 | 96.8 | -0.07 | 102.3 | 0.30 |
| CYT997 (Lexibulin) | 917111-44-5 | free base | Microtubule Associat | 55.5 | -1.31 | 52.5 | -1.22 | 43.3 | -2.34 | 27.7 | -2.06 |
| CZC24832 | 1159824-67-5 | free base | PI3K | 84.4 | -0.08 | 106.1 | 0.73 | 82.1 | -0.69 | 100.5 | 0.24 |
| Dabrafenib (GSK2118436) | 1195765-45-7 | free base | Raf | 96.4 | 0.42 | 113.9 | 1.01 | 197.9 | 4.22 | 128.4 | 1.13 |
| Daclatasvir (BMS-790052) | 1009119-64-5 | free base | HCV Protease | 149.9 | 2.69 | 106.5 | 0.75 | 116.7 | 0.78 | 60.9 | -1.01 |
| Dacomitinib (PF299804, PF299) | 1110813-31-4 | free base | EGFR | 113.4 | 1.14 | 114.1 | 1.02 | 101.9 | 0.14 | 87.5 | -0.17 |
| Dalcatrapib (JTT-705, RO4607381) | 211513-37-0 | free base | CETP | 69.3 | -0.72 | 115.3 | 1.07 | 121.7 | 0.99 | 139.4 | 1.48 |
| Danoprevir (ITMN-191) | 850876-88-9 | free base | HCV Protease | 120.2 | 1.43 | 114.2 | 1.02 | 104.6 | 0.26 | 107.3 | 0.46 |
| Danusertib (PHA-739358) | 827318-97-8 | free base | c-RET,FGFR,Bcr-Abl,Aurora Kinase | | | 71.1 | -0.54 | 41.3 | -2.43 | 61.0 | -1.01 |
| Dapagliflozin | 461432-26-8 | free base | SGLT | 117.4 | 1.31 | 91.9 | 0.21 | 109.6 | 0.47 | 93.2 | 0.01 |
| Dapivirine (TMC120) | 244767-67-7 | free base | Reverse Transcriptase | 82.9 | -0.15 | 57.1 | -1.05 | 127.4 | 1.23 | 121.5 | 0.91 |
| Dapoxetine HCl | 129938-20-1 | hydrochloride | 5-HT Receptor | 100.2 | 0.59 | 60.2 | -0.94 | 106.2 | 0.33 | 133.9 | 1.30 |
| DAPT (GSI-IX) | 208255-80-5 | free base | Gamma-secretase,Beta Amyloid | 110.0 | 1.00 | 79.4 | -0.24 | 81.5 | -0.72 | 116.7 | 0.76 |
| Darapladib (SB-480848) | 356057-34-6 | free base | Phospholipase (e.g. | 86.3 | 0.00 | 65.3 | -0.75 | 100.4 | 0.08 | 124.4 | 1.00 |
| Darifenacin HBr | 133099-07-7 | HBr | AChR | 93.2 | 0.29 | 53.4 | -1.18 | 114.1 | 0.66 | 113.8 | 0.66 |
| Darunavir Ethanolate | 635728-49-3 | ethanolate | HIV Protease | 88.0 | 0.07 | 114.7 | 1.05 | 94.4 | -0.17 | 97.1 | 0.14 |
| Dasatinib | 302962-49-8 | free base | Bcr-Abl,c-Kit,Src | 110.5 | 1.02 | 117.1 | 1.13 | 115.3 | 0.72 | 93.6 | 0.02 |
| Daunorubicin HCl | 23541-50-6 | hydrochloride | Telomerase | 25.9 | -2.57 | 65.0 | -0.76 | 117.3 | 0.80 | 12.1 | -2.56 |
| DBeQ | 177355-84-9 | free base | p97 | 77.2 | -0.39 | 109.0 | 0.83 | | | 77.4 | -0.49 |
| DCC-2036 (Rebastinib) | 1020172-07-9 | free base | Bcr-Abl | 69.1 | -0.73 | 62.7 | -0.85 | 83.4 | -0.64 | 124.1 | 0.99 |
| Decamethonium Bromide | 541-22-0 | bromide | AChR | 93.5 | 0.30 | 116.6 | 1.11 | 112.4 | 0.59 | 89.1 | -0.12 |
| Decitabine | 2353-33-5 | free base | DNA Methyltransferase | 90.2 | 0.16 | 102.1 | 0.58 | 104.4 | 0.25 | 58.6 | -1.08 |

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| Degrasyn (WP1130) | 856243-80-6 | free base | DUB,Bcr-Abl | 102.3 | 0.67 | 93.0 | 0.26 | 92.6 | -0.25 | 77.6 | -0.48 |
| Dehydroepiandrosterone (DHEA) | 53-43-0 | free base | Androgen Receptor | 109.2 | 0.97 | 102.7 | 0.61 | 125.8 | 1.16 | 127.8 | 1.11 |
| Deltarasin | 1440898-61-2 | free base | PDE | 85.4 | -0.04 | 92.8 | 0.25 | | | 86.9 | -0.19 |
| Demeclocycline HCl | 64-73-3 | Salt | Others | 67.8 | -0.79 | 117.3 | 1.14 | 77.0 | -0.91 | 107.4 | 0.46 |
| Desloratadine | 100643-71-8 | free base | Histamine Receptor | 115.8 | 1.24 | 116.0 | 1.09 | 109.3 | 0.46 | 95.0 | 0.07 |
| Desvenlafaxine | 93413-62-8 | free base | 5-HT Receptor | 97.9 | 0.49 | 67.2 | -0.68 | 90.4 | -0.34 | 126.3 | 1.06 |
| Desvenlafaxine Succinate | 386750-22-7 | succinate | 5-HT Receptor | 155.8 | 2.94 | 117.8 | 1.16 | 100.2 | 0.07 | 122.2 | 0.93 |
| Detomidine HCl | 90038-01-0 | hydrochloride | Adrenergic Receptor | 121.2 | 1.47 | 114.8 | 1.05 | 94.5 | -0.17 | 125.9 | 1.05 |
| Dexamethasone (DHAP) | 50-02-2 | free base | Autophagy,IL Receptor | 81.8 | -0.20 | 115.5 | 1.07 | 160.5 | 2.64 | 68.3 | -0.78 |
| Dexmedetomidine | 113775-47-6 | free base | Adrenergic Receptor | 89.9 | 0.15 | 118.1 | 1.17 | 115.9 | 0.74 | 124.9 | 1.02 |
| Dibucaine HCl | 61-12-1 | free base | Sodium Channel | 76.2 | -0.43 | 118.0 | 1.16 | 101.0 | 0.11 | 137.9 | 1.43 |
| Diclofenac Sodium | 15307-79-6 | sodium | COX | 93.1 | 0.28 | 117.5 | 1.14 | 104.6 | 0.26 | 105.3 | 0.39 |
| Dicoumarol | 66-76-2 | free base | Others | 74.6 | -0.50 | 79.7 | -0.23 | 77.6 | -0.89 | 128.0 | 1.12 |
| Didanosine | 69655-05-6 | free base | Reverse Transcriptase | 95.4 | 0.38 | 114.6 | 1.04 | 79.4 | -0.81 | 98.6 | 0.18 |
| Dienogest | 65928-58-7 | free base | Estrogen/progestogen Receptor | 93.0 | 0.28 | 86.3 | 0.01 | 108.3 | 0.42 | 92.4 | -0.01 |
| Digoxin | 20830-75-5 | free base | Sodium Channel | 40.0 | -1.97 | 15.9 | -2.55 | 22.6 | -3.22 | 16.0 | -2.43 |
| Dinaciclib (SCH727965) | 779353-01-4 | free base | CDK | 51.5 | -1.48 | 24.7 | -2.23 | 26.3 | -3.07 | 14.6 | -2.48 |
| Diphenamil Methylsulfate | 62-97-5 | methylsulfate | AChR | 92.6 | 0.26 | 50.3 | -1.30 | 102.1 | 0.16 | 123.8 | 0.98 |
| Diphenidol HCl | 3254-89-5 | Salt | AChR | 88.3 | 0.08 | 68.3 | -0.64 | 90.1 | -0.36 | 106.2 | 0.42 |
| Divalproex Sodium | 76584-70-8 | sodium | Autophagy | 98.9 | 0.53 | 110.1 | 0.88 | 102.9 | 0.19 | 93.1 | 0.01 |
| DMH1 | 1206711-16-1 | free base | BMP | 85.5 | -0.04 | 69.4 | -0.61 | | | 135.1 | 1.34 |
| DMXAA (Vadimezan) | 117570-53-3 | free base | VDA | 96.5 | 0.43 | 115.0 | 1.05 | 104.9 | 0.27 | 81.6 | -0.35 |
| Dolutegravir (GSK1349572) | 1051375-16-6 | free base | Integrase | 75.6 | -0.46 | 112.7 | 0.97 | 124.0 | 1.08 | 121.6 | 0.91 |
| Domperidone | 57808-66-9 | free base | Dopamine Receptor | 113.9 | 1.16 | 116.4 | 1.11 | 123.8 | 1.08 | 116.1 | 0.74 |
| Dopamine HCl | 62-31-7 | hydrochloride | Dopamine Receptor | 100.8 | 0.61 | 59.3 | -0.97 | 118.0 | 0.83 | 124.2 | 0.99 |
| Dovitinib (TKI-258) Dilactic Acid | 852433-84-2 | dilactic Acid | PDGFR,FGFR,c-Kit,FLT3,VEGFR | 52.4 | -1.44 | 57.8 | -1.02 | 95.1 | -0.14 | 17.9 | -2.37 |
| Dovitinib (TKI-258, CHIR-258) | 405169-16-6 | citrate | FGFR,FLT3,c-Kit,VEGFR,PDGFR | 66.7 | -0.84 | 83.4 | -0.10 | 87.0 | -0.49 | 110.8 | 0.57 |
| Doxazosin Mesylate | 77883-43-3 | mesylate | Adrenergic Receptor | 78.9 | -0.32 | 53.0 | -1.20 | 115.1 | 0.71 | 105.9 | 0.41 |

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| Doxorubicin (Adriamycin) | 25316-40-9 | hydrochloride | Autophagy,Topoisomerase | 10.7 | -3.21 | 44.5 | -1.51 | 71.7 | -1.14 | 4.4 | -2.80 |
| Doxycycline HCl | 10592-13-9 | hydrochloride | MMP,Others | 90.9 | 0.19 | 107.9 | 0.80 | 83.3 | -0.64 | 120.5 | 0.88 |
| Drospirenone | 67392-87-4 | free base | Estrogen/progestogen Receptor | 103.4 | 0.72 | 115.5 | 1.07 | 100.0 | 0.07 | 85.4 | -0.24 |
| Droxinostat | 99873-43-5 | free base | HDAC | 103.9 | 0.74 | 114.0 | 1.02 | 110.1 | 0.49 | 98.0 | 0.16 |
| Duloxetine HCl | 136434-34-9 | hydrochloride | 5-HT Receptor | 103.5 | 0.72 | 112.3 | 0.96 | 95.2 | -0.14 | 97.0 | 0.13 |
| Dutasteride | 164656-23-9 | free base | 5-alpha Reductase | 97.6 | 0.47 | 89.3 | 0.12 | 107.9 | 0.40 | 95.8 | 0.10 |
| Dynasore | 304448-55-3 | free base | Dynamain | 73.6 | -0.54 | 65.1 | -0.76 | 76.7 | -0.92 | 88.1 | -0.15 |
| Dyphylline | 479-18-5 | free base | PDE | 98.8 | 0.53 | 116.6 | 1.11 | 111.6 | 0.56 | 79.3 | -0.43 |
| E-64 | 66701-25-5 | free base | Cathepsin K | 85.2 | -0.05 | 65.2 | -0.75 | 100.8 | 0.10 | 131.3 | 1.22 |
| Edoxaban | 480449-70-5 | free base | Factor Xa | 154.8 | 2.90 | 107.2 | 0.77 | 107.8 | 0.40 | 94.1 | 0.04 |
| EHop-016 | 1380432-32-5 | free base | Rac | 100.0 | 0.57 | 115.1 | 1.06 | 104.6 | 0.26 | 84.4 | -0.27 |
| EHT 1864 | 754240-09-0 | Salt | Rho | 84.1 | -0.10 | 95.6 | 0.35 | 107.4 | 0.38 | 67.4 | -0.81 |
| Elesclomol (STA-4783) | 488832-69-5 | free base | HSP (e.g. HSP90) | 96.8 | 0.44 | 117.1 | 1.13 | 89.3 | -0.39 | 71.0 | -0.69 |
| Eletriptan HBr | 177834-92-3 | HBr | 5-HT Receptor | 92.6 | 0.26 | 117.8 | 1.16 | 114.7 | 0.69 | 101.3 | 0.27 |
| Elvitegravir (GS-9137, JTK-303) | 697761-98-1 | free base | Integrase | 94.5 | 0.34 | 116.3 | 1.10 | 106.1 | 0.32 | 105.3 | 0.39 |
| Embelin | 550-24-3 | free base | IAP | 100.4 | 0.59 | 116.5 | 1.11 | 89.4 | -0.39 | 129.0 | 1.15 |
| Empagliflozin (BI 10773) | 864070-44-0 | free base | SGLT | 91.9 | 0.23 | 70.7 | -0.56 | 108.0 | 0.40 | 96.7 | 0.12 |
| Emtricitabine | 143491-57-0 | free base | Reverse Transcriptase | 97.0 | 0.45 | 114.5 | 1.03 | 87.3 | -0.47 | 91.7 | -0.03 |
| Enalapril Maleate | 76095-16-4 | maleate | RAAS | 93.6 | 0.30 | 113.1 | 0.98 | 103.5 | 0.22 | 92.2 | -0.02 |
| Enalaprilat Dihydrate | 84680-54-6 | dihydrate | RAAS | 85.0 | -0.06 | 115.0 | 1.05 | 87.3 | -0.47 | 93.5 | 0.02 |
| ENMD-2076 | 934353-76-1 | tartaric acid | Aurora Kinase,FLT3,VEGFR | 62.2 | -1.02 | 100.2 | 0.52 | 71.5 | -1.14 | 81.1 | -0.37 |
| Entacapone | 130929-57-6 | free base | Histone Methyltransferase | 94.8 | 0.36 | 84.9 | -0.04 | 91.7 | -0.29 | 123.3 | 0.96 |
| Entinostat (MS-275) | 209783-80-2 | free base | HDAC | 50.1 | -1.54 | 94.5 | 0.31 | 106.0 | 0.32 | 2.1 | -2.87 |
| Enzalutamide (MDV3100) | 915087-33-1 | free base | Androgen Receptor | 98.7 | 0.52 | 93.0 | 0.26 | 113.5 | 0.64 | 65.0 | -0.88 |
| Enzastaurin (LY317615) | 170364-57-5 | free base | PKC | 71.3 | -0.64 | 74.7 | -0.41 | 72.3 | -1.11 | 119.5 | 0.85 |
| Epiandrosterone | 481-29-8 | free base | Androgen Receptor,Estrogen Receptor | 85.1 | -0.06 | 113.6 | 1.00 | 106.3 | 0.33 | 113.2 | 0.64 |
| Epinephrine Bitartrate | 51-42-3 | bitartrate | Adrenergic Receptor | 88.5 | 0.09 | 106.4 | 0.74 | 127.0 | 1.21 | 99.4 | 0.21 |
| Epinephrine HCl | 55-31-2 | hydrochloride | Adrenergic Receptor | 84.7 | -0.07 | 58.8 | -0.99 | 115.4 | 0.72 | 111.6 | 0.60 |

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| Epirubicin HCl | 56390-09-1 | hydrochloride | Topoisomerase | 15.6 | -3.00 | 53.5 | -1.18 | 67.3 | -1.32 | 3.5 | -2.83 |
| EPZ004777 | 1338466-77-5 | free base | Histone Methyltransferase | 79.6 | -0.29 | 67.9 | -0.66 | 110.6 | 0.52 | 69.6 | -0.73 |
| EPZ5676 | 1380288-87-8 | free base | Histone Methyltransferase | 103.6 | 0.73 | 73.8 | -0.44 | 99.4 | 0.04 | 88.4 | -0.14 |
| EPZ-6438 | 1403254-99-8 | free base | Histone Methyltransferase | 67.6 | -0.80 | 113.8 | 1.01 | | | 82.2 | -0.34 |
| Equol | 531-95-3 | free base | Estrogen/progestogen Receptor | 117.9 | 1.33 | 93.7 | 0.28 | 97.8 | -0.03 | 110.4 | 0.56 |
| Erastin | 571203-78-6 | free base | Ferroptosis | 159.8 | 3.11 | 90.0 | 0.15 | | | 93.3 | 0.02 |
| Erlotinib HCl (OSI-744) | 183319-69-9 | hydrochloride | Autophagy,EGFR | 86.6 | 0.01 | 68.4 | -0.64 | 92.8 | -0.24 | 114.0 | 0.67 |
| Escitalopram Oxalate | 219861-08-2 | oxalate | 5-HT Receptor | 80.2 | -0.26 | 117.2 | 1.13 | 106.7 | 0.35 | 128.9 | 1.14 |
| ESI-09 | 263707-16-0 | free base | Others | 107.3 | 0.88 | 92.8 | 0.25 | 105.7 | 0.31 | 83.2 | -0.31 |
| Esomeprazole Sodium | 161796-78-7 | free base | ATPase | 108.8 | 0.95 | 115.1 | 1.06 | 88.1 | -0.44 | 118.9 | 0.83 |
| Estradiol Benzoate | 50-50-0 | free base | Others | 132.1 | 1.93 | 116.2 | 1.10 | 106.6 | 0.35 | 42.1 | -1.61 |
| Estradiol Cypionate | 313-06-4 | free base | Estrogen/progestogen | 88.4 | 0.08 | 117.5 | 1.14 | 107.7 | 0.39 | 158.2 | 2.07 |
| Estradiol valerate | 979-32-8 | free base | Estrogen/progestogen Receptor | 96.3 | 0.42 | 97.6 | 0.42 | 111.2 | 0.54 | 87.8 | -0.16 |
| Estriol | 50-27-1 | free base | Estrogen/progestogen Receptor | 81.3 | -0.21 | 117.5 | 1.14 | 123.6 | 1.07 | 108.4 | 0.49 |
| Estrone | 53-16-7 | free base | Estrogen/progestogen Receptor | 98.8 | 0.53 | 114.2 | 1.03 | 96.9 | -0.07 | 90.9 | -0.06 |
| Ethinodiol diacetate | 297-76-7 | free base | Estrogen/progestogen Receptor | 115.5 | 1.23 | 115.4 | 1.07 | 110.4 | 0.51 | 126.6 | 1.07 |
| Etizolam | 40054-69-1 | free base | Others | 104.3 | 0.76 | 118.3 | 1.17 | 100.0 | 0.07 | 122.0 | 0.92 |
| Etodolac | 41340-25-4 | free base | COX | 95.8 | 0.40 | 52.3 | -1.22 | 138.3 | 1.69 | 77.3 | -0.49 |
| Etomidate | 33125-97-2 | free base | GABA Receptor | 99.9 | 0.57 | 66.9 | -0.69 | 115.6 | 0.73 | 99.7 | 0.22 |
| Etoposide | 33419-42-0 | free base | Topoisomerase | 75.9 | -0.45 | 69.7 | -0.59 | 89.7 | -0.37 | 11.8 | -2.57 |
| ETP-46464 | 1345675-02-6 | free base | mTOR,ATM/ATR | 61.8 | -1.04 | 57.3 | -1.04 | 87.8 | -0.45 | 75.1 | -0.56 |
| Etravirine (TMC125) | 269055-15-4 | free base | Reverse Transcriptase | 119.7 | 1.41 | 115.3 | 1.07 | 115.0 | 0.70 | 98.3 | 0.17 |
| EUK 134 | 81065-76-1 | free base | Beta Amyloid | 64.8 | -0.92 | 114.7 | 1.04 | 83.8 | -0.62 | 104.4 | 0.37 |
| Evacetrapib (LY2484595) | 1186486-62-3 | free base | CETP | 81.9 | -0.19 | 70.3 | -0.57 | 106.9 | 0.36 | 78.2 | -0.46 |
| Everolimus (RAD001) | 159351-69-6 | free base | mTOR | 90.1 | 0.15 | 84.0 | -0.07 | 64.7 | -1.44 | 64.2 | -0.91 |
| EX 527 (Selisistat) | 49843-98-3 | free base | Sirtuin | 89.0 | 0.11 | 51.4 | -1.26 | 105.4 | 0.29 | 94.9 | 0.07 |
| Exemestane | 107868-30-4 | free base | Aromatase | 96.5 | 0.43 | 102.2 | 0.59 | 120.5 | 0.94 | 94.7 | 0.06 |

| | | | | | | | | | | | |
|--------------------------------|--------------|---------------|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Famotidine | 76824-35-6 | free base | Histamine Receptor | 98.1 | 0.50 | 116.0 | 1.09 | 103.3 | 0.20 | 99.6 | 0.22 |
| Fasudil (HA-1077) HCl | 105628-07-7 | hydrochloride | ROCK, Autophagy | 161.3 | 3.17 | 116.0 | 1.09 | 109.0 | 0.45 | 98.1 | 0.17 |
| Felodipine | 72509-76-3 | free base | Calcium Channel | 93.3 | 0.29 | 71.1 | -0.54 | 106.8 | 0.35 | 149.7 | 1.80 |
| Ferrostatin-1 (Fer-1) | 347174-05-4 | free base | Ferroptosis | 72.9 | -0.57 | 112.9 | 0.98 | | | 111.6 | 0.59 |
| Fesoterodine Fumarate | 286930-03-8 | fumarate | AChR | 108.6 | 0.94 | 59.9 | -0.95 | 90.8 | -0.32 | 80.9 | -0.38 |
| Fexofenadine HCl | 153439-40-8 | hydrochloride | Histamine Receptor | 87.6 | 0.05 | 116.9 | 1.12 | 108.6 | 0.43 | 94.9 | 0.07 |
| FG-4592 | 808118-40-3 | free base | HIF | 111.8 | 1.08 | 105.4 | 0.71 | 92.0 | -0.27 | 111.0 | 0.58 |
| FH535 | 108409-83-2 | free base | Wnt/beta-catenin | 103.7 | 0.73 | 114.7 | 1.04 | 100.8 | 0.10 | 87.9 | -0.16 |
| Filgotinib (GLPG0634) | 1206161-97-8 | free base | JAK | 69.6 | -0.71 | 64.0 | -0.80 | 83.3 | -0.64 | 123.8 | 0.98 |
| Finasteride | 98319-26-7 | free base | 5-alpha Reductase | 84.5 | -0.08 | 106.1 | 0.73 | 118.3 | 0.84 | 64.4 | -0.90 |
| Fingolimod (FTY720) HCl | 162359-56-0 | hydrochloride | S1P Receptor | 75.2 | -0.47 | 86.3 | 0.01 | 78.5 | -0.85 | 128.8 | 1.14 |
| Flavopiridol HCl | 131740-09-5 | hydrochloride | CDK | 54.1 | -1.37 | 20.7 | -2.37 | 31.6 | -2.84 | 21.8 | -2.25 |
| Flavoxate HCl | 3717-88-2 | hydrochloride | AChR | 91.5 | 0.21 | 96.9 | 0.40 | 96.6 | -0.08 | 121.7 | 0.92 |
| FLI-06 | 313967-18-9 | free base | Notch | 82.8 | -0.15 | 116.7 | 1.12 | 110.4 | 0.51 | 99.9 | 0.23 |
| Flumazenil | 78755-81-4 | free base | GABA Receptor | 78.2 | -0.35 | 114.6 | 1.04 | 111.4 | 0.55 | 95.4 | 0.08 |
| Flumequine | 42835-25-6 | free base | Topoisomerase | 114.1 | 1.17 | 114.8 | 1.05 | 117.2 | 0.79 | 142.0 | 1.56 |
| Flunarizine 2HCl | 30484-77-6 | 2HCl | Calcium Channel | 97.3 | 0.46 | 115.5 | 1.07 | 105.6 | 0.30 | 131.4 | 1.22 |
| Flunixin Meglumine | 42461-84-7 | meglumine | COX | 102.2 | 0.67 | 109.9 | 0.87 | 91.9 | -0.28 | 95.6 | 0.09 |
| Fluoxetine HCl | 56296-78-7 | hydrochloride | 5-HT Receptor | 86.0 | -0.02 | 116.0 | 1.09 | 92.8 | -0.24 | 70.1 | -0.72 |
| Flutamide | 13311-84-7 | free base | Androgen Receptor | 100.2 | 0.58 | 117.1 | 1.13 | 82.9 | -0.66 | 127.8 | 1.11 |
| Fluvastatin Sodium | 93957-55-2 | sodium | HMG-CoA Reductase | 101.3 | 0.63 | 116.7 | 1.11 | 102.9 | 0.19 | 86.7 | -0.19 |
| Fluvoxamine maleate | 61718-82-9 | maleate | 5-HT Receptor | 100.9 | 0.62 | 49.3 | -1.33 | 87.6 | -0.46 | 78.5 | -0.45 |
| Foretinib (GSK1363089) | 849217-64-7 | free base | VEGFR,c-Met | 48.0 | -1.63 | 76.2 | -0.35 | 65.5 | -1.40 | 67.1 | -0.81 |
| Formestane | 566-48-3 | free base | Aromatase | 117.1 | 1.30 | 94.9 | 0.32 | 90.6 | -0.33 | 88.1 | -0.15 |
| Formoterol Hemifumarate | 43229-80-7 | fumarate | Adrenergic Receptor | 106.2 | 0.84 | 115.7 | 1.08 | 109.5 | 0.47 | 91.5 | -0.04 |
| Forskolin | 66575-29-9 | free base | cAMP | 123.6 | 1.58 | 90.9 | 0.18 | 90.7 | -0.33 | 128.0 | 1.12 |
| Fostamatinib (R788) | 901119-35-5 | free base | Syk | 68.1 | -0.78 | 57.2 | -1.05 | 108.5 | 0.43 | 92.9 | 0.00 |
| FPH2 (BRD-9424) | 957485-64-2 | free base | Others | 84.1 | -0.10 | 96.6 | 0.39 | 104.0 | 0.23 | 83.2 | -0.30 |
| Fulvestrant | 129453-61-8 | free base | Estrogen/progestogen | 108.2 | 0.92 | 83.2 | -0.10 | 128.1 | 1.26 | 103.1 | 0.32 |

| | | | Receptor | | | | | | | | |
|-------------------------------|--------------|-------------|-------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Gabexate Mesylate | 56974-61-9 | mesylate | Proteasome | 101.1 | 0.62 | 115.6 | 1.08 | 93.5 | -0.21 | 98.7 | 0.19 |
| Galeterone | 851983-85-2 | free base | P450 (e.g. CYP17),Androgen Receptor | 94.8 | 0.36 | 65.1 | -0.76 | 104.6 | 0.26 | 118.4 | 0.81 |
| Gallamine Triethiodide | 65-29-2 | Iodine salt | AChR | 90.8 | 0.19 | 116.9 | 1.12 | 113.6 | 0.64 | 101.8 | 0.28 |
| Ganetespib (STA-9090) | 888216-25-9 | free base | HSP (e.g. HSP90) | 57.0 | -1.25 | 31.9 | -1.97 | 49.4 | -2.09 | 39.6 | -1.69 |
| GDC-0068 | 1001264-89-6 | free base | Akt | 64.6 | -0.92 | 110.2 | 0.88 | 89.5 | -0.38 | 106.0 | 0.42 |
| GDC-0152 | 873652-48-3 | free base | IAP | 85.7 | -0.03 | 115.4 | 1.07 | 82.9 | -0.66 | 115.8 | 0.73 |
| GDC-0349 | 1207360-89-1 | free base | mTOR | 54.1 | -1.37 | 101.1 | 0.55 | 65.3 | -1.41 | 105.7 | 0.41 |
| GDC-0879 | 905281-76-7 | free base | Raf | 121.1 | 1.47 | 115.1 | 1.06 | 151.1 | 2.24 | 98.3 | 0.17 |
| GDC-0941 | 957054-30-7 | free base | PI3K | 57.3 | -1.24 | 84.1 | -0.07 | 74.1 | -1.03 | 83.3 | -0.30 |
| GDC-0980 (RG7422) | 1032754-93-0 | free base | mTOR,PI3K | 55.6 | -1.31 | 43.7 | -1.54 | 78.7 | -0.84 | 76.6 | -0.51 |
| Gefitinib (ZD1839) | 184475-35-2 | free base | EGFR | 86.6 | 0.01 | 116.5 | 1.11 | 96.6 | -0.08 | 118.1 | 0.80 |
| Geldanamycin | 30562-34-6 | free base | HSP (e.g. HSP90),Autophagy | 37.4 | -2.08 | 38.8 | -1.72 | 49.0 | -2.10 | 41.5 | -1.63 |
| Gemcitabine | 95058-81-4 | free base | Autophagy,DNA/RNA Synthesis | 75.6 | -0.46 | 81.8 | -0.15 | 65.2 | -1.41 | 16.5 | -2.42 |
| Genistein | 446-72-0 | free base | Topoisomerase,EGFR | 83.2 | -0.14 | 116.5 | 1.11 | 125.8 | 1.16 | 68.8 | -0.76 |
| Gestodene | 60282-87-3 | free base | Estrogen/progestogen Receptor | 88.1 | 0.07 | 55.9 | -1.09 | 92.8 | -0.24 | 68.4 | -0.77 |
| GF109203X | 133052-90-1 | free base | PKC | 67.5 | -0.80 | 74.6 | -0.41 | | | 91.7 | -0.04 |
| Gimeracil | 103766-25-2 | free base | Dehydrogenase | 98.3 | 0.50 | 115.9 | 1.09 | 85.8 | -0.54 | 95.1 | 0.07 |
| Ginkgolide A | 15291-75-5 | free base | GABA Receptor | 100.2 | 0.58 | 116.1 | 1.09 | 103.2 | 0.20 | 89.4 | -0.11 |
| Ginkgolide B | 15291-77-7 | free base | PAFR | 99.3 | 0.55 | 116.8 | 1.12 | 106.7 | 0.35 | 98.4 | 0.18 |
| Givinostat (ITF2357) | 732302-99-7 | chloride | HDAC | 44.6 | -1.77 | 37.8 | -1.75 | 46.5 | -2.21 | -0.4 | -2.95 |
| Gliclazide | 21187-98-4 | free base | Potassium Channel | 83.2 | -0.14 | 69.3 | -0.61 | 97.5 | -0.04 | 109.7 | 0.54 |
| Glimepiride | 93479-97-1 | free base | DPP-4 | 86.3 | -0.01 | 96.2 | 0.37 | 134.3 | 1.52 | 104.4 | 0.37 |
| Gliquidone | 33342-05-1 | free base | Potassium Channel | 98.3 | 0.50 | 80.1 | -0.22 | 112.1 | 0.58 | 130.5 | 1.19 |
| GNE-0877 | 1374828-69-9 | free base | LRRK2 | 83.9 | -0.10 | 116.0 | 1.09 | 98.1 | -0.02 | 142.0 | 1.56 |
| GNE-7915 | 1351761-44-8 | free base | LRRK2 | 109.4 | 0.97 | 54.5 | -1.14 | 98.9 | 0.02 | 76.2 | -0.53 |
| GNE-9605 | 1536200-31-3 | free base | LRRK2 | 82.2 | -0.18 | 111.2 | 0.92 | 115.4 | 0.72 | 78.2 | -0.46 |

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|----------------------------|--------------|---------------|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| GNF-2 | 778270-11-4 | free base | Bcr-Abl | 82.0 | -0.19 | 49.4 | -1.33 | 102.7 | 0.18 | 98.1 | 0.17 |
| GNF-5 | 778277-15-9 | free base | Bcr-Abl | 85.4 | -0.04 | 60.7 | -0.92 | 72.4 | -1.11 | 82.8 | -0.32 |
| Go 6983 | 133053-19-7 | free base | PKC | 71.2 | -0.64 | 44.4 | -1.51 | 79.8 | -0.79 | 98.0 | 0.16 |
| Golgicide A | 1139889-93-2 | free base | ATPase | 86.6 | 0.01 | 117.1 | 1.13 | 93.6 | -0.21 | 101.1 | 0.26 |
| Golvatinib (E7050) | 928037-13-2 | free base | VEGFR,c-Met | 72.6 | -0.59 | 65.1 | -0.76 | 115.9 | 0.74 | 95.1 | 0.07 |
| GS-9973 | 1229208-44-9 | free base | Syk | 95.3 | 0.38 | 78.9 | -0.26 | 110.7 | 0.52 | 121.6 | 0.91 |
| GSK J4 HCl | 1373423-53-0 | hydrochloride | Histone demethylases | 102.2 | 0.67 | 89.1 | 0.11 | 80.0 | -0.78 | 43.6 | -1.56 |
| GSK1059615 | 958852-01-2 | free base | PI3K,mTOR | 45.2 | -1.75 | 47.8 | -1.39 | 81.7 | -0.71 | 42.0 | -1.61 |
| GSK1292263 | 1032823-75-8 | free base | GPR | 108.6 | 0.94 | 96.1 | 0.37 | 95.1 | -0.14 | 110.1 | 0.55 |
| GSK1838705A | 1116235-97-2 | free base | IGF-1R,ALK | 42.4 | -1.86 | 48.3 | -1.37 | 91.2 | -0.31 | 96.4 | 0.11 |
| GSK1904529A | 1089283-49-7 | free base | IGF-1R | 90.2 | 0.16 | 62.8 | -0.84 | 81.6 | -0.72 | 127.7 | 1.10 |
| GSK2126458 (GSK458) | 1086062-66-9 | free base | PI3K,mTOR | 33.2 | -2.26 | 32.1 | -1.96 | 55.3 | -1.83 | 14.7 | -2.47 |
| GSK2334470 | 1227911-45-6 | free base | PDK-1 | 75.9 | -0.44 | 99.4 | 0.49 | | | 75.4 | -0.55 |
| GSK256066 | 801312-28-7 | free base | PDE | 93.1 | 0.28 | 46.8 | -1.43 | 133.9 | 1.50 | 94.0 | 0.04 |
| GSK2606414 | 1337531-36-8 | free base | PERK | 77.4 | -0.38 | 63.8 | -0.81 | 101.3 | 0.12 | 75.4 | -0.55 |
| GSK2636771 | 1372540-25-4 | free base | PI3K | 81.9 | -0.19 | 73.7 | -0.45 | 102.9 | 0.19 | 77.8 | -0.47 |
| GSK2656157 | 1337532-29-2 | free base | PERK | 81.2 | -0.22 | 65.5 | -0.75 | 75.6 | -0.97 | 113.0 | 0.64 |
| GSK2656157 | 1337532-29-2 | free base | PERK | 73.6 | -0.54 | 87.7 | 0.06 | 80.2 | -0.78 | 116.5 | 0.75 |
| GSK3787 | 188591-46-0 | free base | PPAR | 88.0 | 0.07 | 110.5 | 0.89 | 105.8 | 0.31 | 75.0 | -0.57 |
| GSK429286A | 864082-47-3 | free base | ROCK | 117.0 | 1.30 | 106.4 | 0.74 | 112.9 | 0.61 | 86.7 | -0.19 |
| GSK461364 | 929095-18-1 | free base | PLK | 76.3 | -0.43 | 49.7 | -1.32 | 58.9 | -1.68 | 45.2 | -1.51 |
| GSK690693 | 937174-76-0 | free base | Akt | 71.1 | -0.65 | 111.2 | 0.92 | 89.8 | -0.37 | 120.1 | 0.86 |
| GSK923295 | 1088965-37-0 | free base | Kinesin | 68.2 | -0.77 | 85.4 | -0.02 | | | 72.8 | -0.63 |
| Guanabenz Acetate | 23256-50-0 | acetate | Adrenergic Receptor | 82.0 | -0.19 | 117.0 | 1.13 | 113.1 | 0.62 | 119.0 | 0.83 |
| GW0742 | 317318-84-6 | free base | PPAR | 71.8 | -0.62 | 66.5 | -0.71 | 112.1 | 0.58 | 156.2 | 2.01 |
| GW2580 | 870483-87-7 | free base | CSF-1R | 82.1 | -0.18 | 83.9 | -0.08 | 100.8 | 0.10 | 84.6 | -0.26 |
| GW3965 HCl | 405911-17-3 | hydrochloride | Liver X Receptor | 80.6 | -0.24 | 92.5 | 0.24 | 117.0 | 0.79 | 108.8 | 0.51 |
| GW4064 | 278779-30-9 | free base | FXR | 90.0 | 0.15 | 115.5 | 1.07 | 115.1 | 0.71 | 118.5 | 0.81 |
| GW5074 | 220904-83-6 | free base | Raf | 93.3 | 0.29 | 90.0 | 0.15 | 113.6 | 0.64 | 99.7 | 0.22 |

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|----------------------------------|--------------|---------------|----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| GW788388 | 452342-67-5 | free base | TGF-beta/Smad | 82.0 | -0.19 | 114.6 | 1.04 | 135.8 | 1.59 | 104.9 | 0.38 |
| GW842166X | 666260-75-9 | free base | Cannabinoid Receptor | 92.7 | 0.27 | 114.5 | 1.04 | 117.5 | 0.81 | 119.7 | 0.85 |
| GW9508 | 885101-89-3 | free base | GPR | 83.5 | -0.12 | 64.4 | -0.78 | 79.6 | -0.80 | 142.9 | 1.59 |
| GW9662 | 22978-25-2 | free base | PPAR | 86.1 | -0.01 | 70.2 | -0.57 | 108.6 | 0.43 | 107.7 | 0.47 |
| GZD824 | 1421783-64-3 | mesylate | Bcr-Abl | 57.5 | -1.22 | 66.9 | -0.70 | | | 106.8 | 0.44 |
| H 89 2HCl | 130964-39-5 | 2HCl | PKA | 92.5 | 0.26 | 62.9 | -0.84 | 100.3 | 0.08 | 84.2 | -0.27 |
| HA14-1 | 65673-63-4 | free base | Bcl-2 | 56.7 | -1.26 | 49.7 | -1.32 | 63.0 | -1.51 | 118.1 | 0.80 |
| HER2-Inhibitor-1 | 937265-83-3 | free base | HER2,EGFR | 111.1 | 1.05 | 93.4 | 0.27 | 111.3 | 0.55 | 137.5 | 1.42 |
| Hesperadin | 422513-13-1 | free base | Aurora Kinase | 53.9 | -1.38 | 52.0 | -1.24 | 43.7 | -2.32 | 70.5 | -0.71 |
| Hesperetin | 520-33-2 | free base | Histamine Receptor,TGF-beta/Smad | 114.9 | 1.20 | 54.0 | -1.16 | 100.0 | 0.06 | 88.2 | -0.14 |
| Hexestrol | 84-16-2 | free base | Estrogen/progestogen Receptor | 97.2 | 0.46 | 117.3 | 1.14 | 124.3 | 1.10 | 129.9 | 1.17 |
| Histamine 2HCl | 56-92-8 | hydrochloride | Histamine Receptor | 91.9 | 0.23 | 81.8 | -0.15 | 82.3 | -0.69 | 90.2 | -0.08 |
| HJC0350 | 885434-70-8 | free base | Others | 106.0 | 0.83 | 97.7 | 0.43 | 102.0 | 0.15 | 105.5 | 0.40 |
| HMN-214 | 173529-46-9 | free base | PLK | 57.5 | -1.22 | 77.6 | -0.31 | 70.7 | -1.18 | 46.4 | -1.47 |
| HO-3867 | 1172133-28-6 | free base | STAT | 111.3 | 1.06 | 96.1 | 0.37 | 111.8 | 0.56 | 56.9 | -1.14 |
| Homatropine Bromide | 51-56-9 | bromide | AChR | 96.8 | 0.44 | 64.4 | -0.78 | 116.7 | 0.77 | 94.9 | 0.07 |
| Homatropine Methylbromide | 80-49-9 | Methylbromide | AChR | 88.3 | 0.08 | 89.5 | 0.13 | 107.8 | 0.40 | 128.1 | 1.12 |
| Honokiol | 35354-74-6 | free base | MEK,Akt | 107.4 | 0.89 | 62.3 | -0.86 | 99.2 | 0.03 | 82.1 | -0.34 |
| HS-173 | 1276110-06-5 | free base | PI3K | 91.2 | 0.20 | 57.3 | -1.05 | 69.5 | -1.23 | 48.3 | -1.41 |
| HSP990 (NVP-HSP990) | 934343-74-5 | free base | HSP (e.g. HSP90) | 50.2 | -1.53 | 32.0 | -1.96 | | | 38.9 | -1.71 |
| Hydroxyzine 2HCl | 2192-20-3 | hydrochloride | Histamine Receptor | 112.8 | 1.12 | 115.0 | 1.06 | 115.5 | 0.72 | 94.9 | 0.06 |
| Hyoscyamine | 101-31-5 | free base | AChR | 88.1 | 0.07 | 112.9 | 0.98 | 102.4 | 0.17 | 119.2 | 0.84 |
| I-BET151 (GSK1210151A) | 1300031-49-5 | free base | Epigenetic Reader Domain | 41.9 | -1.89 | 89.1 | 0.11 | 77.7 | -0.88 | 44.2 | -1.54 |
| I-BET-762 | 1260907-17-2 | free base | Epigenetic Reader Domain | 51.0 | -1.50 | 55.0 | -1.13 | | | 43.6 | -1.56 |
| Ibrutinib (PCI-32765) | 936563-96-1 | free base | BTK | 79.4 | -0.30 | 47.2 | -1.41 | 117.8 | 0.82 | 117.7 | 0.79 |
| Ibuprofen | 15687-27-1 | free base | COX | 124.3 | 1.61 | 81.4 | -0.17 | 108.2 | 0.41 | 78.6 | -0.45 |
| Ibutilide Fumarate | 122647-32-9 | fumarate | Sodium Channel | 150.6 | 2.72 | 110.7 | 0.90 | 98.4 | 0.00 | 105.0 | 0.38 |
| Icariin | 489-32-7 | free base | PDE | 108.0 | 0.92 | 73.1 | -0.47 | 93.2 | -0.22 | 115.4 | 0.72 |

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|-------------------------------------|--------------|----------------|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| ICG-001 | 780757-88-2 | free base | Wnt/beta-catenin | 75.7 | -0.45 | 67.1 | -0.69 | 109.7 | 0.48 | 49.8 | -1.36 |
| Icotinib | 610798-31-7 | free base | EGFR | 82.4 | -0.17 | 114.8 | 1.05 | 95.3 | -0.13 | 97.0 | 0.13 |
| Idarubicin HCl | 57852-57-0 | hydrochloride | Topoisomerase | 4.8 | -3.46 | 4.9 | -2.95 | 23.3 | -3.19 | 2.1 | -2.87 |
| IEM 1754 dihydrobroMide | 162831-31-4 | dihydrobroMide | GluR,5-HT Receptor | 76.2 | -0.43 | 60.2 | -0.94 | 121.8 | 0.99 | 99.5 | 0.21 |
| Ifenprodil Tartrate | 23210-58-4 | tartrate | GluR | 103.4 | 0.72 | 115.8 | 1.08 | 104.8 | 0.27 | 117.4 | 0.78 |
| IKK-16 (IKK Inhibitor VII) | 873225-46-8 | free base | IkB/IKK | 90.8 | 0.18 | 47.7 | -1.39 | 113.9 | 0.65 | 84.6 | -0.26 |
| Ilomastat (GM6001, Galardin) | 142880-36-2 | free base | MMP | 80.9 | -0.23 | 113.5 | 1.00 | | | 86.9 | -0.19 |
| IM-12 | 1129669-05-1 | free base | GSK-3 | 81.4 | -0.21 | 70.6 | -0.56 | 101.0 | 0.11 | 112.3 | 0.62 |
| Imatinib (STI571) | 152459-95-5 | free base | PDGFR | 88.9 | 0.10 | 52.2 | -1.23 | 156.4 | 2.46 | 116.2 | 0.74 |
| Imatinib Mesylate (STI571) | 220127-57-1 | mesylate | c-Kit,Bcr-Abl,PDGFR | 91.2 | 0.20 | 116.9 | 1.12 | 102.5 | 0.17 | 121.2 | 0.90 |
| IMD 0354 | 978-62-1 | free base | IkB/IKK | 65.7 | -0.88 | 57.2 | -1.05 | 113.1 | 0.62 | 77.8 | -0.47 |
| Imidapril HCl | 89396-94-1 | free base | RAAS | 126.9 | 1.72 | 114.3 | 1.03 | 94.5 | -0.17 | 122.2 | 0.93 |
| INCB024360 | 914471-09-3 | free base | IDO | 89.4 | 0.13 | 106.9 | 0.76 | 75.7 | -0.97 | 88.0 | -0.15 |
| Indacaterol Maleate | 753498-25-8 | maleate | Adrenergic Receptor | 94.5 | 0.34 | 109.1 | 0.84 | 103.7 | 0.22 | 119.6 | 0.85 |
| Indirubin | 479-41-4 | free base | GSK-3 | 104.9 | 0.78 | 72.8 | -0.48 | 89.7 | -0.37 | 102.3 | 0.30 |
| INH1 | 313553-47-8 | free base | Microtubule Associat | 101.3 | 0.63 | 79.2 | -0.25 | 87.3 | -0.47 | 100.7 | 0.25 |
| INH6 | 1001753-24-7 | free base | Microtubule Associat | 85.5 | -0.04 | 92.1 | 0.22 | 99.7 | 0.05 | 88.3 | -0.14 |
| Iniparib (BSI-201) | 160003-66-7 | free base | PARP | 92.9 | 0.28 | 101.2 | 0.55 | 94.7 | -0.16 | 92.2 | -0.02 |
| INK 128 (MLN0128) | 1224844-38-5 | free base | mTOR | 38.0 | -2.05 | 39.3 | -1.70 | 35.2 | -2.69 | 28.9 | -2.02 |
| INO-1001 | 3544-24-9 | free base | PARP | 108.9 | 0.95 | 117.4 | 1.14 | 111.7 | 0.56 | 92.6 | -0.01 |
| IOWH032 | 1191252-49-9 | free base | CFTR | 80.4 | -0.26 | 93.8 | 0.28 | 82.0 | -0.70 | 103.2 | 0.33 |
| IOX1 | 5852-78-8 | free base | Histone demethylases | 74.9 | -0.49 | 104.0 | 0.66 | | | 88.2 | -0.15 |
| IOX2 | 931398-72-0 | free base | HIF | 92.0 | 0.24 | 110.4 | 0.89 | 99.0 | 0.02 | 107.4 | 0.46 |
| IPA-3 | 42521-82-4 | free base | PAK | 84.1 | -0.10 | 75.8 | -0.37 | | | 80.1 | -0.40 |
| IPI-145 (INK1197) | 1201438-56-3 | free base | PI3K | 81.3 | -0.22 | 114.8 | 1.05 | 98.5 | 0.00 | 110.6 | 0.56 |
| IPI-145 (INK1197) | 1201438-56-3 | free base | PI3K | 89.3 | 0.12 | 100.2 | 0.52 | 91.8 | -0.28 | 111.5 | 0.59 |
| Irinotecan | 97682-44-5 | free base | Topoisomerase | 56.7 | -1.26 | 99.2 | 0.48 | 108.9 | 0.44 | 28.6 | -2.03 |
| Irinotecan HCl Trihydrate | 136572-09-3 | hydrate | Topoisomerase | 66.3 | -0.85 | 49.1 | -1.34 | 93.8 | -0.20 | 77.8 | -0.48 |

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|----------------------------------|--------------|---------------|---------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Irsogladine | 57381-26-7 | free base | PDE,AChR | 106.4 | 0.85 | 115.5 | 1.07 | 98.2 | -0.01 | 84.2 | -0.27 |
| Isoprenaline HCl | 51-30-9 | hydrochloride | Adrenergic Receptor | 76.2 | -0.43 | 116.2 | 1.10 | 120.7 | 0.94 | 104.0 | 0.35 |
| Isotretinoin | 4759-48-2 | free base | Hydroxylase | 91.2 | 0.20 | 63.4 | -0.82 | 121.2 | 0.96 | 93.1 | 0.01 |
| Ispinesib (SB-715992) | 336113-53-2 | free base | Kinesin | 46.3 | -1.70 | 91.6 | 0.21 | 45.9 | -2.23 | 32.4 | -1.91 |
| Isradipine | 75695-93-1 | free base | Calcium Channel | 87.6 | 0.05 | 115.5 | 1.07 | 110.7 | 0.52 | 73.6 | -0.61 |
| IU1 | 314245-33-5 | free base | DUB | 89.3 | 0.12 | 108.7 | 0.82 | | | 121.7 | 0.91 |
| Ivabradine HCl | 148849-67-6 | hydrochloride | Adrenergic Receptor | 98.3 | 0.50 | 75.4 | -0.38 | 88.9 | -0.41 | 129.4 | 1.16 |
| Ivacaftor (VX-770) | 873054-44-5 | free base | CFTR | 98.4 | 0.51 | 113.0 | 0.98 | 113.9 | 0.66 | 95.7 | 0.09 |
| IWP-2 | 686770-61-6 | free base | Wnt/beta-catenin | 129.7 | 1.83 | 88.1 | 0.07 | | | 114.5 | 0.69 |
| IWP-L6 | 1427782-89-5 | free base | Wnt/beta-catenin | 79.2 | -0.31 | 54.3 | -1.15 | 97.9 | -0.03 | 79.1 | -0.44 |
| IWR-1-endo | 1127442-82-3 | free base | Wnt/beta-catenin | 106.0 | 0.83 | 100.2 | 0.52 | | | 113.7 | 0.66 |
| JNJ-1661010 | 681136-29-8 | free base | FAAH | 93.5 | 0.30 | 113.4 | 0.99 | 124.3 | 1.10 | 113.4 | 0.65 |
| JNJ-26854165 (Serdemetan) | 881202-45-5 | free base | p53,E3 Ligase | 105.6 | 0.81 | 108.5 | 0.82 | 130.6 | 1.36 | 86.7 | -0.19 |
| JNJ-38877605 | 943540-75-8 | free base | c-Met | 130.2 | 1.86 | 111.7 | 0.93 | 113.9 | 0.65 | 64.2 | -0.91 |
| JNJ-7706621 | 443797-96-4 | free base | CDK,Aurora Kinase | 71.9 | -0.62 | 74.2 | -0.43 | 82.9 | -0.66 | 56.0 | -1.17 |
| JNJ-7777120 | 459168-41-3 | free base | Histamine Receptor | 91.1 | 0.20 | 99.7 | 0.50 | 101.8 | 0.14 | 97.2 | 0.14 |
| JNK Inhibitor IX | 312917-14-9 | free base | JNK | 61.3 | -1.06 | 49.7 | -1.32 | 45.2 | -2.26 | 33.8 | -1.87 |
| JNK-IN-8 | 1410880-22-6 | free base | JNK | 91.8 | 0.23 | 71.2 | -0.54 | 79.7 | -0.80 | 120.4 | 0.87 |
| JSH-23 | 749886-87-1 | free base | NF-κB | 80.6 | -0.25 | 102.8 | 0.61 | 99.6 | 0.05 | 115.5 | 0.72 |
| JTC-801 | 244218-51-7 | hydrochloride | Opioid Receptor | 83.8 | -0.11 | 61.3 | -0.90 | 124.1 | 1.09 | 135.7 | 1.36 |
| K02288 | 1431985-92-0 | free base | TGF-beta/Smad | 74.2 | -0.52 | 116.4 | 1.11 | 125.4 | 1.15 | 79.8 | -0.41 |
| Ketanserin | 74050-98-9 | free base | 5-HT Receptor | 116.3 | 1.27 | 106.9 | 0.76 | 96.5 | -0.09 | 84.9 | -0.25 |
| Ketoconazole | 65277-42-1 | free base | P450 (e.g. CYP17) | 99.4 | 0.55 | 74.6 | -0.42 | 111.3 | 0.55 | 69.1 | -0.75 |
| Ketoprofen | 22071-15-4 | free base | COX | 83.2 | -0.14 | 115.3 | 1.06 | 99.5 | 0.04 | 78.8 | -0.44 |
| Ketorolac | 74103-07-4 | tromethamine | COX | 84.3 | -0.09 | 115.1 | 1.06 | 89.4 | -0.39 | 94.0 | 0.04 |
| Ketotifen Fumarate | 34580-14-8 | fumarate | Histamine Receptor | 98.9 | 0.53 | 115.4 | 1.07 | 101.3 | 0.12 | 147.0 | 1.72 |
| Ki16198 | 355025-13-7 | free base | LPA Receptor | 101.2 | 0.63 | 73.0 | -0.47 | 97.5 | -0.04 | 94.9 | 0.07 |
| Ki16425 | 355025-24-0 | free base | LPA Receptor | 93.8 | 0.31 | 55.9 | -1.09 | 104.7 | 0.27 | 89.1 | -0.12 |
| Ki8751 | 228559-41-9 | free base | PDGFR,c-Kit,VEGFR | 71.3 | -0.64 | 50.8 | -1.28 | 53.3 | -1.92 | 35.0 | -1.83 |

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|---|--------------|-----------|------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| KN-62 | 127191-97-3 | free base | Others | 121.2 | 1.47 | 105.8 | 0.72 | 105.2 | 0.29 | 103.3 | 0.33 |
| KN-93 Phosphate | 1188890-41-6 | free base | Others | 86.7 | 0.01 | 76.1 | -0.36 | 97.4 | -0.05 | 83.9 | -0.28 |
| KPT-185 | 1333151-73-7 | free base | CRM1 | 58.5 | -1.18 | 38.5 | -1.73 | | | 3.7 | -2.82 |
| KPT-276 | 1421919-75-6 | free base | CRM1 | 68.7 | -0.75 | 76.9 | -0.33 | | | 7.8 | -2.69 |
| KPT-330 | 1393477-72-9 | free base | CRM1 | 59.6 | -1.13 | 49.7 | -1.32 | | | 3.6 | -2.83 |
| K-Ras(G12C) inhibitor 6 | N/A | free base | Ras | 105.9 | 0.83 | 116.9 | 1.12 | 100.5 | 0.08 | 84.3 | -0.27 |
| K-Ras(G12C) inhibitor 9 | 1469337-91-4 | free base | Rho | 116.1 | 1.26 | 88.8 | 0.10 | 109.7 | 0.48 | 99.6 | 0.21 |
| KRN 633 | 286370-15-8 | free base | PDGFR,VEGFR | 80.4 | -0.26 | 116.0 | 1.09 | 133.5 | 1.49 | 97.8 | 0.16 |
| KU-0063794 | 938440-64-3 | free base | mTOR | 70.6 | -0.67 | 96.5 | 0.38 | 94.0 | -0.19 | 59.1 | -1.07 |
| KU-55933 (ATM Kinase Inhibitor) | 587871-26-9 | free base | ATM/ATR | 100.4 | 0.59 | 99.2 | 0.48 | 104.5 | 0.25 | 88.0 | -0.15 |
| KU-60019 | 925701-49-1 | free base | ATM/ATR | 96.9 | 0.45 | 115.1 | 1.06 | 122.3 | 1.01 | 79.0 | -0.44 |
| KW-2449 | 1000669-72-6 | free base | Aurora Kinase,Bcr-Abl,FLT3 | 85.6 | -0.03 | 55.1 | -1.12 | 91.7 | -0.29 | 74.2 | -0.59 |
| KW-2478 | 819812-04-9 | free base | HSP (e.g. HSP90) | 53.9 | -1.38 | 62.3 | -0.86 | 49.5 | -2.08 | 53.7 | -1.24 |
| KX2-391 | 897016-82-9 | free base | Src | 45.9 | -1.72 | 50.2 | -1.30 | 59.7 | -1.65 | 26.7 | -2.09 |
| KY02111 | 1118807-13-8 | free base | Wnt/beta-catenin | 88.7 | 0.10 | 88.2 | 0.08 | | | 117.7 | 0.79 |
| Labetalol HCl | 32780-64-6 | Salt | Adrenergic Receptor | 84.8 | -0.07 | 82.4 | -0.13 | 80.3 | -0.77 | 93.6 | 0.03 |
| Lacidipine | 103890-78-4 | free base | Calcium Channel | 80.6 | -0.25 | 116.2 | 1.10 | 87.9 | -0.45 | 123.0 | 0.96 |
| L-Adrenaline | 51-43-4 | free base | Adrenergic Receptor | 105.1 | 0.79 | 50.8 | -1.28 | 134.2 | 1.52 | 117.5 | 0.78 |
| Lafutidine | 118288-08-7 | free base | Histamine Receptor | 100.1 | 0.58 | 116.3 | 1.10 | 96.6 | -0.08 | 141.7 | 1.55 |
| Lamivudine | 134678-17-4 | free base | Reverse Transcriptase | 107.6 | 0.90 | 114.9 | 1.05 | 109.2 | 0.45 | 76.5 | -0.52 |
| Lamotrigine | 84057-84-1 | free base | Sodium Channel,5-HT Receptor | 114.9 | 1.21 | 119.2 | 1.21 | 110.6 | 0.52 | 115.3 | 0.71 |
| Lansoprazole | 103577-45-3 | free base | Proton Pump | 78.8 | -0.32 | 70.8 | -0.55 | 101.8 | 0.14 | 94.9 | 0.07 |
| Lapatinib (GW-572016) Ditosylate | 388082-77-7 | ditosylat | HER2,EGFR | 95.7 | 0.39 | 115.7 | 1.08 | 93.2 | -0.22 | 109.2 | 0.52 |
| LAQ824 (Dacinostat) | 404951-53-7 | free base | HDAC | 2.3 | -3.56 | 21.6 | -2.34 | 17.2 | -3.45 | 1.9 | -2.88 |
| Laquinimod | 248281-84-7 | free base | Others | 109.5 | 0.98 | 109.0 | 0.84 | 95.9 | -0.11 | 106.0 | 0.42 |
| LB42708 | 226929-39-1 | free base | Ftase | 72.3 | -0.60 | 57.8 | -1.03 | 60.4 | -1.62 | 77.6 | -0.48 |
| LDC000067 | 1073485-20-7 | free base | CDK | 95.9 | 0.40 | 115.4 | 1.07 | 92.2 | -0.27 | 77.1 | -0.50 |
| LDE225 (NVP-LDE225,Erismodegib) | 956697-53-3 | free base | Hedgehog/Smoothened | 81.3 | -0.21 | 81.4 | -0.17 | 93.4 | -0.22 | 117.1 | 0.77 |

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|-------------------------------------|--------------|---------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| LDK378 | 1032900-25-6 | free base | ALK | 65.0 | -0.91 | 80.1 | -0.21 | 72.2 | -1.11 | 120.3 | 0.87 |
| LDN-212854 | 1432597-26-6 | free base | BMP | 76.8 | -0.41 | 109.5 | 0.85 | | | 110.0 | 0.54 |
| LDN-57444 | 668467-91-2 | free base | DUB | 81.3 | -0.22 | 64.9 | -0.77 | | | 112.5 | 0.62 |
| LEE011 | 1211441-98-3 | free base | CDK | 67.0 | -0.82 | 115.8 | 1.08 | 67.3 | -1.32 | 115.8 | 0.73 |
| Lenalidomide (CC-5013) | 191732-72-6 | free base | TNF-alpha | 98.0 | 0.49 | 88.3 | 0.08 | 76.8 | -0.92 | 117.0 | 0.77 |
| Lenvatinib (E7080) | 417716-92-8 | free base | VEGFR | 106.7 | 0.86 | 116.9 | 1.12 | 98.2 | -0.01 | 61.9 | -0.98 |
| Letrozole | 112809-51-5 | free base | Aromatase | 94.1 | 0.33 | 77.5 | -0.31 | 131.6 | 1.41 | 110.1 | 0.55 |
| Leupeptin Hemisulfate | 103476-89-7 | free base | Serine Protease | 77.0 | -0.40 | 83.5 | -0.09 | 97.8 | -0.03 | 82.9 | -0.32 |
| Levodropropizine | 99291-25-5 | free base | Histamine Receptor | 109.5 | 0.98 | 117.4 | 1.14 | 102.4 | 0.17 | 62.7 | -0.95 |
| Levosulpiride | 23672-07-3 | free base | Dopamine Receptor | 106.1 | 0.83 | 98.6 | 0.46 | 92.8 | -0.24 | 134.5 | 1.32 |
| LGK-974 | 1243244-14-5 | free base | Wnt/beta-catenin | 68.5 | -0.76 | 70.6 | -0.56 | | | 141.6 | 1.55 |
| LGX818 | 1269440-17-6 | free base | RAF | 86.0 | -0.02 | 62.1 | -0.87 | | | 120.8 | 0.89 |
| Licofelone | 156897-06-2 | free base | COX | 115.5 | 1.23 | 112.5 | 0.96 | 84.6 | -0.59 | 116.3 | 0.74 |
| Lidocaine | 137-58-6 | free base | Histamine Receptor | 82.6 | -0.16 | 53.9 | -1.17 | 89.2 | -0.39 | 88.0 | -0.15 |
| Linagliptin | 668270-12-0 | free base | DPP-4 | 97.3 | 0.46 | 64.8 | -0.77 | 116.9 | 0.78 | 117.9 | 0.79 |
| Linifanib (ABT-869) | 796967-16-3 | free base | CSF-1R,PDGFR,VEGFR | 102.5 | 0.68 | 109.2 | 0.84 | 84.3 | -0.60 | 122.0 | 0.92 |
| Lomeguatrib | 192441-08-0 | free base | DNA Methyltransferase | 75.5 | -0.46 | 70.5 | -0.56 | 102.9 | 0.19 | 130.5 | 1.19 |
| Lomitapide | 182431-12-5 | free base | Others | 77.1 | -0.39 | 66.6 | -0.71 | 102.6 | 0.18 | 131.0 | 1.21 |
| Lonafarnib | 193275-84-2 | free base | Transferase | 94.5 | 0.34 | 105.9 | 0.72 | 94.4 | -0.17 | 92.4 | -0.01 |
| Loperamide HCl | 34552-83-5 | hydrochloride | Opioid Receptor,Autophagy | 103.3 | 0.71 | 115.2 | 1.06 | 121.7 | 0.99 | 123.2 | 0.96 |
| Lopinavir | 192725-17-0 | free base | HIV Protease | 100.6 | 0.60 | 50.5 | -1.29 | 122.8 | 1.03 | 75.0 | -0.57 |
| Loratadine | 79794-75-5 | free base | Histamine Receptor | 85.8 | -0.03 | 51.1 | -1.27 | 125.9 | 1.17 | 81.8 | -0.35 |
| Lorcaserin HCl | 846589-98-8 | hydrochloride | 5-HT Receptor | 103.2 | 0.71 | 112.4 | 0.96 | 94.9 | -0.15 | 89.8 | -0.10 |
| Lornoxicam | 70374-39-9 | free base | COX | 99.0 | 0.53 | 115.4 | 1.07 | 101.1 | 0.11 | 127.9 | 1.11 |
| Losartan Potassium (DuP 753) | 124750-99-8 | potassium | RAAS | 82.9 | -0.15 | 109.5 | 0.85 | 121.6 | 0.98 | 86.2 | -0.21 |
| Losmapimod (GW856553X) | 585543-15-3 | free base | p38 MAPK | 75.3 | -0.47 | 62.1 | -0.87 | | | 105.0 | 0.39 |
| Lovastatin | 75330-75-5 | free base | HMG-CoA Reductase | 84.6 | -0.08 | 63.3 | -0.82 | 91.6 | -0.29 | 124.5 | 1.00 |
| Loxistatin Acid (E-64C) | 76684-89-4 | free base | Cysteine protease | 93.3 | 0.29 | 116.7 | 1.12 | 90.9 | -0.32 | 85.3 | -0.24 |
| Lumiracoxib | 220991-20-8 | free base | COX | 101.9 | 0.66 | 67.2 | -0.68 | 114.1 | 0.66 | 104.2 | 0.36 |

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|---------------------------------------|--------------|-----------------|-------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Luteolin | 491-70-3 | free base | PDE | 113.9 | 1.16 | 110.2 | 0.88 | 99.8 | 0.06 | 82.3 | -0.33 |
| LY2157299 | 700874-72-2 | free base | TGF-beta/Smad | 100.1 | 0.58 | 54.8 | -1.14 | 100.2 | 0.07 | 118.0 | 0.80 |
| LY2228820 | 862507-23-1 | mesylate | p38 MAPK | 111.0 | 1.04 | 114.4 | 1.03 | 105.0 | 0.28 | 63.5 | -0.93 |
| LY2603618 | 911222-45-2 | free base | Chk | 63.9 | -0.95 | 40.7 | -1.65 | 127.6 | 1.24 | 35.2 | -1.83 |
| LY2784544 | 1229236-86-5 | free base | JAK | 82.7 | -0.16 | 53.5 | -1.18 | 65.9 | -1.38 | 77.1 | -0.50 |
| LY2811376 | 1194044-20-6 | free base | Beta Amyloid,Gamma-secretase | 90.7 | 0.18 | 104.0 | 0.65 | 85.4 | -0.56 | 82.4 | -0.33 |
| LY2835219 | 1231930-82-7 | mesylate | CDK | 57.3 | -1.23 | 71.6 | -0.52 | | | 76.9 | -0.50 |
| LY294002 | 154447-36-6 | free base | Autophagy,PI3K | 109.0 | 0.96 | 115.9 | 1.09 | 100.8 | 0.10 | 88.6 | -0.13 |
| LY411575 | 209984-57-6 | free base | Gamma-secretase | 115.5 | 1.23 | 64.6 | -0.78 | 111.0 | 0.53 | 108.4 | 0.50 |
| M344 | 251456-60-7 | free base | HDAC | 35.4 | -2.16 | 48.2 | -1.38 | 74.0 | -1.04 | 2.9 | -2.85 |
| Macitentan | 441798-33-0 | free base | Endothelin Receptor | 81.2 | -0.22 | 61.0 | -0.91 | 105.3 | 0.29 | 129.2 | 1.15 |
| Manidipine | 89226-50-6 | free base | Calcium Channel | 94.6 | 0.34 | 115.8 | 1.08 | 148.5 | 2.13 | 125.6 | 1.04 |
| Manidipine 2HCl | 89226-75-5 | dihydrochloride | Calcium Channel | 99.1 | 0.54 | 112.7 | 0.97 | 122.4 | 1.02 | 117.9 | 0.79 |
| Maprotiline HCl | 10347-81-6 | hydrochloride | Adrenergic Receptor | 96.3 | 0.42 | 109.9 | 0.87 | 111.5 | 0.56 | 123.1 | 0.96 |
| Maraviroc | 376348-65-1 | free base | CCR | 91.4 | 0.21 | 114.6 | 1.04 | 109.8 | 0.48 | 98.9 | 0.19 |
| Masitinib (AB1010) | 790299-79-5 | free base | PDGFR,c-Kit | 102.8 | 0.69 | 114.5 | 1.04 | 81.2 | -0.73 | 96.7 | 0.12 |
| MC1568 | 852475-26-4 | free base | HDAC | 140.8 | 2.30 | 94.8 | 0.32 | 114.8 | 0.69 | 74.3 | -0.59 |
| Mdivi-1 | 338967-87-6 | free base | Dynamin | 79.3 | -0.30 | 61.8 | -0.88 | | | 101.1 | 0.26 |
| ME0328 | 1445251-22-8 | free base | PARP | 102.9 | 0.70 | 116.3 | 1.10 | 92.8 | -0.24 | 89.8 | -0.10 |
| Meclofenamate Sodium | 6385-02-0 | free base | COX | 106.8 | 0.86 | 117.2 | 1.14 | 93.1 | -0.23 | 97.1 | 0.14 |
| Medetomidine HCl | 86347-15-1 | hydrochloride | Adrenergic Receptor | 90.4 | 0.17 | 119.1 | 1.20 | 104.1 | 0.24 | 113.1 | 0.64 |
| Medroxyprogesterone acetate | 71-58-9 | free base | Estrogen/progestogen Receptor | 89.4 | 0.13 | 114.8 | 1.05 | 123.9 | 1.08 | 93.0 | 0.01 |
| Mefenamic Acid | 61-68-7 | free base | COX | 97.8 | 0.48 | 107.9 | 0.80 | 100.8 | 0.10 | 113.7 | 0.66 |
| Mefloquine HCl | 51773-92-3 | Salt | Others | 83.5 | -0.12 | 81.0 | -0.18 | 78.7 | -0.84 | 139.9 | 1.49 |
| Megestrol Acetate | 595-33-5 | acetate | Estrogen Receptor,Androgen Receptor | 83.6 | -0.12 | 61.7 | -0.88 | 106.6 | 0.34 | 82.2 | -0.34 |
| MEK162 (ARRY-162, ARRY-438162) | 606143-89-9 | free base | MEK | 91.3 | 0.21 | 53.8 | -1.17 | 50.7 | -2.03 | 82.4 | -0.33 |
| Memantine HCl | 41100-52-1 | hydrochloride | AMPA Receptor-kainate | 96.4 | 0.42 | 116.9 | 1.12 | 101.4 | 0.13 | 124.8 | 1.01 |

| | | | Receptor-NMDA Receptor | | | | | | | | |
|--------------------------------|--------------|-----------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Methazolamide | 554-57-4 | free base | Carbonic Anhydrase | 84.4 | -0.09 | 118.3 | 1.17 | 109.4 | 0.46 | 126.3 | 1.06 |
| Methotrexate | 59-05-2 | free base | DHFR | 82.3 | -0.17 | 63.3 | -0.82 | 97.1 | -0.06 | 75.6 | -0.54 |
| Methscopolamine | 155-41-9 | bromide | AChR | 120.3 | 1.43 | 104.1 | 0.66 | 104.7 | 0.26 | 126.8 | 1.08 |
| Metoclopramide HCl | 7232-21-5 | Salt | Dopamine Receptor | 100.4 | 0.59 | 82.9 | -0.11 | 82.9 | -0.66 | 132.1 | 1.24 |
| Metoprolol Tartrate | 392-17-7 | tartrate | Adrenergic Receptor | 93.8 | 0.31 | 71.8 | -0.52 | 116.2 | 0.75 | 94.6 | 0.06 |
| MG-132 | 133407-82-6 | free base | Proteasome | 2.4 | -3.56 | 4.0 | -2.98 | 33.5 | -2.76 | 13.4 | -2.52 |
| MGCD-265 | 875337-44-3 | free base | Tie-2,VEGFR,c-Met | 99.5 | 0.56 | 51.5 | -1.25 | 149.6 | 2.17 | 78.0 | -0.47 |
| MI-2 (MALT1 inhibitor) | 1047953-91-2 | free base | Others | 83.4 | -0.13 | 65.3 | -0.75 | 91.9 | -0.28 | 61.9 | -0.98 |
| Mianserin HCl | 21535-47-7 | hydrochloride | Histamine Receptor | 122.4 | 1.52 | 64.8 | -0.77 | 109.3 | 0.46 | 76.1 | -0.53 |
| Mifepristone | 84371-65-3 | free base | Estrogen/progestogen Receptor | 98.5 | 0.51 | 85.9 | 0.00 | 117.5 | 0.81 | 98.6 | 0.18 |
| Miliciclib (PHA-848125) | 802539-81-7 | free base | CDK | 65.1 | -0.90 | 66.2 | -0.72 | 66.8 | -1.35 | 72.8 | -0.63 |
| Milrinone | 78415-72-2 | free base | ATPase,PDE | 96.5 | 0.43 | 116.6 | 1.11 | 125.7 | 1.16 | 129.3 | 1.16 |
| Mirabegron | 223673-61-8 | free base | Adrenergic Receptor | 92.1 | 0.24 | 87.2 | 0.04 | 109.5 | 0.47 | 123.5 | 0.97 |
| MK-0752 | 471905-41-6 | free base | Gamma-secretase,Beta Amyloid | 114.4 | 1.19 | 91.4 | 0.20 | 114.0 | 0.66 | 116.1 | 0.74 |
| MK-1775 | 955365-80-7 | free base | Wee1 | 86.8 | 0.02 | 24.7 | -2.23 | 94.7 | -0.16 | 34.7 | -1.84 |
| MK-2048 | 869901-69-9 | free base | Integrase | 79.1 | -0.31 | 114.2 | 1.03 | 134.1 | 1.51 | 103.8 | 0.35 |
| MK-2206 2HCl | 1032350-13-2 | dihydrochloride | Akt | 54.4 | -1.35 | 113.2 | 0.99 | 94.3 | -0.18 | 99.7 | 0.22 |
| MK-2461 | 917879-39-1 | free base | c-Met,PDGFR,FGFR | 77.3 | -0.39 | 114.4 | 1.03 | 105.9 | 0.31 | 115.4 | 0.71 |
| MK-2866 (GTX-024) | 841205-47-8 | free base | Androgen Receptor | 118.0 | 1.34 | 116.1 | 1.09 | 115.2 | 0.71 | 66.5 | -0.83 |
| MK-5108 (VX-689) | 1010085-13-8 | free base | Aurora Kinase | 44.6 | -1.77 | 51.6 | -1.25 | 68.8 | -1.26 | 89.2 | -0.11 |
| MK-801 (Dizocilpine) | 77086-21-6 | free base | GluR | 84.8 | -0.07 | 49.5 | -1.33 | 114.3 | 0.67 | 107.0 | 0.45 |
| MK-8245 | 1030612-90-8 | free base | Dehydrogenase | 104.1 | 0.75 | 57.0 | -1.05 | 105.0 | 0.28 | 96.8 | 0.13 |
| MK-8745 | 885325-71-3 | free base | Aurora Kinase | 116.0 | 1.25 | 103.9 | 0.65 | 58.5 | -1.70 | 90.8 | -0.06 |
| MK-8776 (SCH 900776) | 891494-63-6 | free base | CDK,Chk | 68.1 | -0.78 | 52.7 | -1.21 | 123.4 | 1.06 | 50.0 | -1.36 |
| ML130 (Nodinitib-1) | 799264-47-4 | free base | NOD1 | 89.1 | 0.11 | 74.7 | -0.41 | 103.2 | 0.20 | 102.3 | 0.30 |
| ML133 HCl | 1222781-70-5 | hydrochloride | Potassium Channel | 70.9 | -0.66 | 61.9 | -0.88 | 127.7 | 1.24 | 134.1 | 1.31 |
| ML167 | 1285702-20-6 | free base | CDK | 90.4 | 0.17 | 65.0 | -0.76 | 101.2 | 0.11 | 112.2 | 0.61 |

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|---|--------------|-----------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| ML323 | 1572414-83-5 | free base | DUB | 63.9 | -0.95 | 51.6 | -1.25 | 101.7 | 0.14 | 80.4 | -0.39 |
| ML347 | 1062368-49-3 | free base | BMP | 73.4 | -0.55 | 55.8 | -1.10 | | | 128.2 | 1.12 |
| MLN2238 | 1072833-77-2 | free base | Proteasome | 4.2 | -3.48 | 4.0 | -2.98 | 52.5 | -1.95 | 2.8 | -2.85 |
| MLN8054 | 869363-13-3 | free base | Aurora Kinase | 60.2 | -1.11 | 73.2 | -0.47 | 64.4 | -1.45 | 66.6 | -0.83 |
| MLN9708 | 1201902-80-8 | free base | Proteasome | 3.7 | -3.50 | 4.2 | -2.97 | 52.2 | -1.96 | 2.4 | -2.86 |
| MM-102 | 1417329-24-8 | free base | Histone Methyltransferase | 80.3 | -0.26 | 115.5 | 1.07 | 103.1 | 0.20 | 103.3 | 0.33 |
| MNS (3,4-Methylenedioxy-β-nitrostyrene, MDBN) | 1485-00-3 | free base | p97 | 106.3 | 0.84 | 116.9 | 1.12 | 95.3 | -0.14 | 124.0 | 0.99 |
| Mocetinostat (MGCD0103) | 726169-73-9 | free base | HDAC | 38.4 | -2.03 | 66.8 | -0.70 | 91.4 | -0.30 | 0.0 | -2.94 |
| Moclobemide (Ro 111163) | 71320-77-9 | free base | MAO | 94.8 | 0.36 | 80.9 | -0.19 | 114.5 | 0.68 | 111.5 | 0.59 |
| Moexipril HCl | 82586-52-5 | hydrochloride | RAAS | 119.1 | 1.38 | 114.0 | 1.02 | 102.6 | 0.17 | 130.3 | 1.19 |
| Mosapride Citrate | 112885-42-4 | citrate | 5-HT Receptor | 86.1 | -0.01 | 72.8 | -0.48 | 105.0 | 0.28 | 103.9 | 0.35 |
| Motesanib Diphosphate (AMG-706) | 857876-30-3 | diphosphate | VEGFR,PDGFR,c-Kit | 96.1 | 0.41 | 116.0 | 1.09 | 107.7 | 0.39 | 133.3 | 1.28 |
| Moxifloxacin HCl | 186826-86-8 | hydrochloride | Topoisomerase | 83.8 | -0.11 | 64.8 | -0.77 | 110.3 | 0.50 | 96.1 | 0.11 |
| MPEP | 96206-92-7 | free base | GluR | 92.9 | 0.28 | 79.9 | -0.22 | 104.5 | 0.26 | 106.9 | 0.45 |
| MPI-0479605 | 1246529-32-7 | free base | Kinesin | 99.5 | 0.55 | 98.4 | 0.45 | 84.3 | -0.60 | 87.8 | -0.16 |
| MRS 2578 | 711019-86-2 | free base | P2 Receptor | 93.0 | 0.28 | 92.6 | 0.24 | 107.8 | 0.40 | 104.5 | 0.37 |
| Mubritinib (TAK 165) | 366017-09-6 | free base | HER2 | 37.7 | -2.06 | 45.8 | -1.46 | 96.0 | -0.11 | 80.2 | -0.40 |
| Mupirocin | 12650-69-0 | free base | DNA/RNA Synthesis | 106.4 | 0.85 | 118.4 | 1.18 | 96.4 | -0.09 | 125.0 | 1.02 |
| Mycophenolate Mofetil | 128794-94-5 | free base | Dehydrogenase | 55.7 | -1.30 | 63.2 | -0.83 | 86.4 | -0.51 | 31.1 | -1.96 |
| N6022 | 1208315-24-5 | free base | Others | 75.5 | -0.46 | 67.9 | -0.66 | 74.7 | -1.01 | 73.2 | -0.62 |
| Nabumetone | 42924-53-8 | free base | COX | 99.5 | 0.55 | 116.7 | 1.12 | 102.1 | 0.15 | 119.3 | 0.84 |
| Nafamostat Mesylate | 82956-11-4 | mesylate | Proteasome | 83.9 | -0.11 | 82.8 | -0.11 | 85.5 | -0.55 | 90.4 | -0.08 |
| Naftopidil | 57149-07-2 | free base | Adrenergic Receptor | 122.9 | 1.55 | 111.6 | 0.93 | 83.3 | -0.64 | 85.9 | -0.22 |
| Naftopidil DiHCl | 57149-08-3 | dihydrochloride | Adrenergic Receptor | 86.4 | 0.00 | 51.2 | -1.26 | 118.3 | 0.84 | 74.5 | -0.58 |
| Naloxone HCl | 357-08-4 | hydrochloride | Opioid Receptor | 79.1 | -0.31 | 118.6 | 1.19 | 109.7 | 0.48 | 147.6 | 1.73 |
| Naltrexone HCl | 16676-29-2 | hydrochloride | Opioid Receptor | 107.2 | 0.88 | 95.0 | 0.33 | 117.8 | 0.82 | 98.2 | 0.17 |
| Naphazoline HCl | 550-99-2 | hydrochloride | Adrenergic Receptor | 95.7 | 0.40 | 116.1 | 1.09 | 114.9 | 0.70 | 93.6 | 0.02 |
| Naproxen | 26159-34-2 | sodium | COX | 91.2 | 0.20 | 115.1 | 1.06 | 105.9 | 0.32 | 75.0 | -0.56 |

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|--|--------------|---------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Naratriptan | 143388-64-1 | free base | 5-HT Receptor | 87.3 | 0.04 | 68.1 | -0.65 | 110.5 | 0.51 | 99.2 | 0.20 |
| Naringenin | 480-41-1 | free base | P450 (e.g. CYP17) | 108.8 | 0.95 | 77.7 | -0.30 | 91.7 | -0.29 | 105.9 | 0.42 |
| Nateglinide | 105816-04-4 | free base | Potassium Channel | 75.5 | -0.46 | 47.6 | -1.40 | 135.7 | 1.58 | 107.2 | 0.46 |
| Nebivolol | 152520-56-4 | hydrochloride | Adrenergic Receptor | 98.1 | 0.50 | 113.6 | 1.00 | 101.9 | 0.14 | 92.4 | -0.01 |
| Necrostatin-1 | 4311-88-0 | free base | TNF-alpha | 88.0 | 0.07 | 79.9 | -0.22 | 97.7 | -0.03 | 76.4 | -0.52 |
| Nefiracetam | 77191-36-7 | free base | GABA Receptor | 91.8 | 0.23 | 116.4 | 1.10 | 106.6 | 0.35 | 143.9 | 1.62 |
| Nelfinavir Mesylate | 159989-65-8 | Salt | HIV Protease | 83.8 | -0.11 | 116.9 | 1.12 | 79.4 | -0.81 | 103.5 | 0.34 |
| Nevirapine | 129618-40-2 | free base | Reverse Transcriptase | 118.9 | 1.38 | 115.6 | 1.08 | 99.4 | 0.04 | 93.1 | 0.01 |
| Nexturastat A | 1403783-31-2 | free base | HDAC | 67.7 | -0.79 | 109.3 | 0.85 | 103.0 | 0.19 | 138.2 | 1.44 |
| NH125 | 278603-08-0 | free base | ELF2 | 69.6 | -0.71 | 59.9 | -0.95 | 113.9 | 0.66 | 22.4 | -2.23 |
| Nicorandil | 65141-46-0 | free base | Potassium Channel | 99.9 | 0.57 | 116.6 | 1.11 | 103.4 | 0.21 | 131.0 | 1.21 |
| Niflumic acid | 4394-00-7 | free base | GABA Receptor | 127.3 | 1.73 | 113.9 | 1.01 | 113.8 | 0.65 | 95.0 | 0.07 |
| Nilotinib (AMN-107) | 641571-10-0 | free base | Bcr-Abl | 75.6 | -0.46 | 88.9 | 0.11 | 120.8 | 0.95 | 79.8 | -0.41 |
| Nilvadipine | 75530-68-6 | free base | Calcium Channel | 78.9 | -0.32 | 105.7 | 0.72 | 117.1 | 0.79 | 102.3 | 0.30 |
| Nimesulide | 51803-78-2 | free base | COX | 93.0 | 0.28 | 115.9 | 1.09 | 84.7 | -0.59 | 97.5 | 0.15 |
| Nimodipine | 66085-59-4 | free base | Calcium Channel,Autophagy | 108.1 | 0.92 | 116.2 | 1.10 | 103.1 | 0.20 | 115.1 | 0.71 |
| Nintedanib (BIBF 1120) | 656247-17-5 | free base | VEGFR,PDGFR,FGFR | 82.7 | -0.16 | 112.6 | 0.97 | 88.5 | -0.42 | 119.2 | 0.84 |
| Nitrendipine | 39562-70-4 | free base | Calcium Channel,Autophagy | 79.0 | -0.32 | 50.0 | -1.31 | 117.0 | 0.79 | 98.4 | 0.18 |
| Nizatidine | 76963-41-2 | free base | Histamine Receptor | 121.6 | 1.49 | 101.6 | 0.57 | 103.6 | 0.22 | 124.8 | 1.01 |
| NLG919 | 1402836-58-1 | free base | IDO | 81.7 | -0.20 | 94.5 | 0.31 | | | 129.0 | 1.15 |
| NMDA (N-Methyl-D-aspartic acid) | 6384-92-5 | free base | GluR | 85.5 | -0.04 | 76.5 | -0.35 | 86.1 | -0.53 | 121.3 | 0.90 |
| NMS-873 | 1418013-75-8 | free base | p97 | 31.4 | -2.33 | 45.1 | -1.49 | 149.9 | 2.18 | 36.0 | -1.80 |
| NMS-E973 | 1253584-84-7 | free base | HSP90 | 51.4 | -1.48 | 42.0 | -1.60 | 44.5 | -2.29 | 36.2 | -1.79 |
| NMS-P937 (NMS1286937) | 1034616-18-6 | free base | PLK | 60.8 | -1.09 | 50.5 | -1.29 | | | 38.5 | -1.72 |
| Nocodazole | 31430-18-9 | free base | Microtubule associated | 48.9 | -1.59 | 85.1 | -0.03 | 65.6 | -1.39 | 27.2 | -2.08 |
| NPS-2143 | 284035-33-2 | free base | CaSR | 106.7 | 0.86 | 113.9 | 1.02 | 106.3 | 0.33 | 104.2 | 0.36 |
| NSC 23766 | 1177865-17-6 | hydrochloride | Rac | 76.0 | -0.44 | 60.9 | -0.91 | 108.8 | 0.44 | 143.5 | 1.60 |
| NSC 319726 | 71555-25-4 | free base | p53 | 52.5 | -1.44 | 47.5 | -1.40 | | | 9.3 | -2.65 |
| NSC 405020 | 7497-07-6 | free base | MMP | 72.0 | -0.61 | 114.3 | 1.03 | 93.7 | -0.20 | 85.5 | -0.23 |

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|--|-------------------------|---------------|---------------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| NSC697923 | 343351-67-7 | free base | E2 | 91.4 | 0.21 | 77.4 | -0.31 | | | 47.0 | -1.45 |
| NU6027 | 220036-08-8 | free base | CDK | 67.4 | -0.80 | 86.5 | 0.02 | | | 88.8 | -0.13 |
| NU7441 (KU-57788) | 503468-95-9 | free base | DNA-PK,PI3K | 88.0 | 0.07 | 60.5 | -0.93 | 126.9 | 1.21 | 92.8 | 0.00 |
| Nutlin-3 | 890090-75-2 | free base | E3 Ligase ,Mdm2 | 73.1 | -0.56 | 92.0 | 0.22 | 68.8 | -1.26 | 98.6 | 0.18 |
| Nutlin-3a | 675576-98-4 | free base | Mdm2 | 59.7 | -1.13 | 66.7 | -0.70 | 81.6 | -0.72 | 83.7 | -0.29 |
| Nutlin-3b | 675576-97-3 | free base | Mdm2 | 72.0 | -0.61 | 67.8 | -0.66 | 94.2 | -0.18 | 78.8 | -0.44 |
| NVP-ADW742 | 475488-23-4 | free base | IGF-1R | 50.5 | -1.52 | 93.3 | 0.27 | 69.6 | -1.23 | 85.6 | -0.23 |
| NVP-AEW541 | 475489-16-8 | free base | IGF-1R | 48.8 | -1.59 | 55.0 | -1.13 | 76.2 | -0.95 | 102.1 | 0.29 |
| NVP-BHG712 | 940310-85-0 | free base | Raf,Src,Bcr-Abl,VEGFR,Ephrin receptor | 105.2 | 0.80 | 57.6 | -1.03 | 94.2 | -0.18 | 79.6 | -0.42 |
| NVP-BSK805 2HCI | 1092499-93-8 | hydrochloride | JAK | 77.4 | -0.38 | 55.0 | -1.13 | 137.0 | 1.64 | 120.0 | 0.86 |
| NVP-BVU972 | 1185763-69-2 | free base | c-Met | 76.2 | -0.43 | 115.4 | 1.07 | 112.3 | 0.59 | 115.2 | 0.71 |
| Obatoclox Mesylate (GX15-070) | 803712-79-0 | mesylate | Bcl-2,Autophagy | 31.0 | -2.35 | 56.4 | -1.08 | 105.8 | 0.31 | 25.4 | -2.14 |
| OC000459 | 851723-84-7,950688-14-9 | free base | GPR | 87.7 | 0.05 | 50.6 | -1.29 | 122.9 | 1.04 | 81.5 | -0.36 |
| Odanacatib (MK-0822) | 603139-19-1 | free base | Cathepsin K | 131.3 | 1.90 | 113.2 | 0.99 | 107.8 | 0.40 | 68.2 | -0.78 |
| OG-L002 | 1357302-64-7 | free base | Histone demethylases | 70.3 | -0.68 | 74.6 | -0.42 | | | 109.5 | 0.53 |
| Olanzapine | 132539-06-1 | free base | 5-HT Receptor,Dopamine Receptor | 80.0 | -0.27 | 55.4 | -1.11 | 120.5 | 0.94 | 103.8 | 0.35 |
| Olaparib (AZD2281, Ku-0059436) | 763113-22-0 | free base | PARP | 89.1 | 0.11 | 109.6 | 0.86 | 109.7 | 0.48 | 102.2 | 0.30 |
| Oligomycin A | 579-13-5 | free base | ATPase | 28.5 | -2.45 | 93.9 | 0.29 | 110.6 | 0.52 | 13.8 | -2.50 |
| Olmesartan Medoxomil | 144689-63-4 | free base | RAAS | 93.1 | 0.28 | 116.0 | 1.09 | 87.6 | -0.46 | 72.0 | -0.66 |
| Olopatadine HCl | 140462-76-6 | hydrochloride | Histamine Receptor | 84.0 | -0.10 | 70.1 | -0.58 | 135.0 | 1.55 | 88.5 | -0.14 |
| Omecamtiv mecarbil (CK-1827452) | 873697-71-3 | free base | ATPase | 103.8 | 0.74 | 69.2 | -0.61 | 123.3 | 1.05 | 128.6 | 1.13 |
| Omeprazole | 73590-58-6 | free base | Autophagy,Proton Pump | 84.7 | -0.07 | 116.3 | 1.10 | 108.7 | 0.44 | 82.9 | -0.32 |
| Ondansetron HCl | 99614-01-4 | hydrochloride | 5-HT Receptor | 93.1 | 0.28 | 114.6 | 1.04 | 108.9 | 0.44 | 101.3 | 0.27 |
| ONX-0914 (PR-957) | 960374-59-8 | free base | Proteasome | 9.7 | -3.25 | 3.4 | -3.00 | | | 0.6 | -2.92 |
| Oprozomib (ONX 0912) | 935888-69-0 | free base | Proteasome | 8.7 | -3.29 | 2.8 | -3.02 | 34.5 | -2.72 | 5.4 | -2.77 |
| Optovin | 348575-88-2 | free base | Others | 72.0 | -0.61 | 113.1 | 0.98 | 98.8 | 0.01 | 113.8 | 0.66 |
| Org 27569 | 868273-06-7 | free base | Cannabinoid Receptor | 130.9 | 1.88 | 104.9 | 0.69 | 122.0 | 1.00 | 94.0 | 0.04 |
| Orphenadrine Citrate | 4682-36-4 | citrate | AChR | 100.4 | 0.59 | 116.1 | 1.09 | 100.5 | 0.08 | 77.5 | -0.48 |

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|-------------------------------------|--------------|---------------|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| OSI-027 | 936890-98-1 | free base | mTOR | 68.5 | -0.76 | 69.3 | -0.61 | 81.7 | -0.71 | 75.6 | -0.54 |
| OSI-420 | 183320-51-6 | hydrochloride | EGFR | 106.9 | 0.87 | 55.3 | -1.11 | 87.7 | -0.46 | 109.1 | 0.52 |
| OSI-906 (Linsitinib) | 867160-71-2 | free base | IGF-1R | 45.9 | -1.71 | 62.5 | -0.85 | 58.1 | -1.71 | 110.7 | 0.57 |
| OSI-930 | 728033-96-3 | free base | c-Kit,CSF-1R,VEGFR | 101.9 | 0.65 | 71.5 | -0.53 | 171.1 | 3.08 | 91.2 | -0.05 |
| Ospemifene | 128607-22-7 | free base | Estrogen/progestogen | 81.9 | -0.19 | 117.4 | 1.14 | 88.1 | -0.44 | 109.6 | 0.53 |
| OSU-03012 (AR-12) | 742112-33-0 | free base | PDK-1 | 226.7 | 5.94 | 109.3 | 0.85 | 96.0 | -0.10 | 96.4 | 0.11 |
| Otilonium Bromide | 26095-59-0 | free base | AChR | 89.3 | 0.12 | 103.1 | 0.62 | 116.3 | 0.76 | 104.4 | 0.37 |
| OTX015 | 202590-98-5 | free base | BET | 30.8 | -2.36 | 47.9 | -1.39 | 51.0 | -2.02 | 12.2 | -2.55 |
| Ouabain | 630-60-4 | free base | Sodium Channel | 41.0 | -1.92 | 12.1 | -2.69 | 25.7 | -3.09 | 20.6 | -2.29 |
| Oxcarbazepine | 28721-07-5 | free base | Sodium Channel | 80.7 | -0.24 | 54.5 | -1.15 | 126.6 | 1.20 | 99.9 | 0.23 |
| Oxiracetam | 62613-82-5 | free base | Others | 76.8 | -0.41 | 78.1 | -0.29 | 84.2 | -0.61 | 103.3 | 0.33 |
| Oxybutynin chloride | 1508-65-2 | chloride | AChR | 89.3 | 0.12 | 119.2 | 1.21 | 98.6 | 0.01 | 119.7 | 0.85 |
| Oxymetazoline HCl | 2315-02-8 | hydrochloride | Adrenergic Receptor | 77.4 | -0.38 | 49.8 | -1.32 | 119.5 | 0.89 | 142.2 | 1.56 |
| Ozagrel | 82571-53-7 | free base | Factor Xa | 91.6 | 0.22 | 58.4 | -1.00 | 148.5 | 2.13 | 137.9 | 1.43 |
| P22077 | 1247819-59-5 | free base | DUB | 70.3 | -0.68 | 73.4 | -0.46 | | | 123.1 | 0.96 |
| P276-00 | 920113-03-7 | hydrochloride | CDK | 24.7 | -2.61 | 32.3 | -1.95 | 70.2 | -1.20 | 27.6 | -2.07 |
| P5091 (P005091) | 882257-11-6 | free base | DUB | 72.3 | -0.60 | 85.2 | -0.03 | | | 93.8 | 0.03 |
| PAC-1 | 315183-21-2 | free base | Caspase | 89.5 | 0.13 | 114.0 | 1.02 | 112.3 | 0.59 | 114.7 | 0.69 |
| Pacritinib (SB1518) | 937272-79-2 | free base | JAK | 75.0 | -0.48 | 67.3 | -0.68 | 103.5 | 0.21 | 91.4 | -0.04 |
| Palbociclib (PD-0332991) HCl | 827022-32-2 | hydrochloride | CDK | 105.6 | 0.81 | 103.0 | 0.62 | 68.0 | -1.29 | 54.2 | -1.22 |
| Palomid 529 (P529) | 914913-88-5 | free base | mTOR | 90.8 | 0.19 | 79.7 | -0.23 | 77.4 | -0.90 | 106.5 | 0.43 |
| Pancuronium dibromide | 15500-66-0 | bromide | AChR | 97.2 | 0.46 | 111.3 | 0.92 | 122.7 | 1.03 | 118.4 | 0.81 |
| Panobinostat (LBH589) | 404950-80-7 | free base | HDAC | 2.4 | -3.56 | 22.2 | -2.32 | 13.8 | -3.60 | 2.4 | -2.87 |
| Paroxetine HCl | 78246-49-8 | hydrochloride | AChR,5-HT Receptor | 140.9 | 2.31 | 112.9 | 0.98 | 111.1 | 0.54 | 121.9 | 0.92 |
| Pazopanib | 444731-52-6 | free base | PDGFR,c-Kit,VEGFR | 122.9 | 1.55 | 116.5 | 1.11 | 157.6 | 2.51 | 117.6 | 0.78 |
| Pazopanib HCl (GW786034 HCl) | 635702-64-6 | hydrochloride | VEGFR,PDGFR,c-Kit | 83.1 | -0.14 | 113.3 | 0.99 | 122.8 | 1.03 | 110.1 | 0.55 |
| PCI-24781 (Abexinostat) | 783355-60-2 | free base | HDAC | 2.6 | -3.55 | 21.5 | -2.35 | 19.5 | -3.36 | 2.5 | -2.86 |
| PCI-34051 | 950762-95-5 | free base | HDAC | 98.1 | 0.49 | 113.3 | 0.99 | 106.5 | 0.34 | 95.4 | 0.08 |
| PD 151746 | 179461-52-0 | free base | Cysteine Protease | 73.6 | -0.54 | 107.1 | 0.77 | 91.6 | -0.29 | 125.0 | 1.02 |

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|--------------------------------------|--------------|-----------------|-------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| PD0325901 | 391210-10-9 | free base | MEK | 84.9 | -0.06 | 30.8 | -2.01 | 50.3 | -2.05 | 109.6 | 0.53 |
| PD123319 | 130663-39-7 | free base | RAAS | 82.7 | -0.16 | 61.6 | -0.89 | | | 95.2 | 0.08 |
| PD128907 HCl | 112960-16-4 | hydrochloride | Dopamine Receptor | 94.9 | 0.36 | 106.9 | 0.76 | 81.2 | -0.73 | 83.5 | -0.29 |
| PD168393 | 194423-15-9 | free base | EGFR | 93.0 | 0.28 | 63.4 | -0.82 | 69.1 | -1.25 | 90.1 | -0.09 |
| PD168393 | 194423-15-9 | free base | EGFR | 72.4 | -0.59 | 102.6 | 0.60 | 74.5 | -1.02 | 98.0 | 0.16 |
| PD173074 | 219580-11-7 | free base | VEGFR,FGFR | 96.3 | 0.42 | 103.3 | 0.63 | 97.1 | -0.06 | 61.4 | -1.00 |
| PD173955 | 260415-63-2 | free base | BCR-ABL | 64.5 | -0.93 | 101.5 | 0.56 | 100.0 | 0.06 | 54.7 | -1.21 |
| PD184352 (CI-1040) | 212631-79-3 | free base | MEK | 93.8 | 0.31 | 57.3 | -1.04 | 44.2 | -2.31 | 91.5 | -0.04 |
| PD318088 | 391210-00-7 | free base | MEK | 87.7 | 0.05 | 30.3 | -2.02 | 51.5 | -1.99 | 82.7 | -0.32 |
| PD98059 | 167869-21-8 | free base | MEK | 77.5 | -0.38 | 109.0 | 0.84 | 122.1 | 1.01 | 75.3 | -0.55 |
| Pefloxacin Mesylate Dihydrate | 149676-40-4 | Mesylate | Topoisomerase | 89.2 | 0.12 | 85.3 | -0.03 | 82.4 | -0.68 | 117.8 | 0.79 |
| Pelitinib (EKB-569) | 257933-82-7 | free base | EGFR | 74.4 | -0.51 | 54.7 | -1.14 | 112.2 | 0.58 | 75.7 | -0.54 |
| Pergolide mesylate | 66104-23-2 | mesylate | Dopamine Receptor | 92.2 | 0.25 | 118.4 | 1.18 | 101.8 | 0.14 | 125.3 | 1.03 |
| PF-00562271 | 939791-38-5 | benzenesulfonic | FAK | 62.6 | -1.01 | 107.3 | 0.78 | 101.5 | 0.13 | 89.1 | -0.12 |
| PF-04217903 | 956905-27-4 | free base | c-Met | 110.8 | 1.03 | 115.1 | 1.06 | 87.2 | -0.48 | 121.9 | 0.92 |
| PF-04620110 | 1109276-89-2 | free base | Transferase | 75.3 | -0.47 | 97.2 | 0.41 | | | 105.2 | 0.39 |
| PF-04691502 | 1013101-36-4 | free base | Akt,mTOR,PI3K | 38.5 | -2.03 | 36.7 | -1.79 | 68.9 | -1.25 | 48.8 | -1.39 |
| PF-04929113 (SNX-5422) | 908115-27-5 | free base | HSP (e.g. HSP90) | 50.3 | -1.53 | 29.2 | -2.07 | 40.3 | -2.47 | 52.3 | -1.28 |
| PF-2545920 | 1292799-56-4 | free base | PDE | 112.9 | 1.12 | 62.2 | -0.87 | 118.5 | 0.85 | 116.2 | 0.74 |
| PF-3758309 | 898044-15-0 | free base | PAK | 66.5 | -0.84 | 36.4 | -1.80 | | | 16.8 | -2.41 |
| PF-3845 | 1196109-52-0 | free base | FAAH | 89.2 | 0.12 | 111.8 | 0.94 | 131.5 | 1.40 | 100.0 | 0.23 |
| PF-4708671 | 1255517-76-0 | free base | S6 Kinase | 100.3 | 0.59 | 100.9 | 0.54 | 108.1 | 0.41 | 106.9 | 0.45 |
| PF-477736 | 952021-60-2 | free base | Chk | 60.4 | -1.10 | 19.2 | -2.43 | 106.3 | 0.33 | 30.6 | -1.97 |
| PF-4981517 | 1390637-82-7 | free base | P450 (e.g. CYP17) | 107.0 | 0.87 | 98.4 | 0.45 | 100.5 | 0.09 | 96.2 | 0.11 |
| PF-5274857 | 1373615-35-0 | free base | Hedgehog/Smoothed | 116.5 | 1.28 | 98.4 | 0.45 | 111.0 | 0.53 | 115.6 | 0.72 |
| PF-543 | 1415562-82-1 | free base | S1P Receptor | 88.2 | 0.08 | 77.4 | -0.31 | | | 121.0 | 0.89 |
| PF-562271 | 717907-75-0 | free base | FAK | 70.1 | -0.69 | 51.6 | -1.25 | 115.7 | 0.73 | 92.0 | -0.03 |
| PF-562271 HCl | N/A | hydrochloride | FAK | 73.1 | -0.56 | 77.8 | -0.30 | 83.3 | -0.64 | 87.5 | -0.17 |

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|---|--------------|---------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| PF-573228 | 869288-64-2 | free base | FAK | 105.0 | 0.79 | 107.6 | 0.78 | 104.0 | 0.24 | 111.4 | 0.59 |
| PFI-1 (PF-6405761) | 1403764-72-6 | free base | Epigenetic Reader Domain | 87.1 | 0.03 | 94.9 | 0.32 | 87.7 | -0.46 | 60.5 | -1.02 |
| PFK15 | 4382-63-2 | free base | Others | 80.9 | -0.23 | 67.5 | -0.67 | 77.2 | -0.90 | 109.2 | 0.52 |
| PH-797804 | 586379-66-0 | free base | p38 MAPK | 81.2 | -0.22 | 114.3 | 1.03 | 118.8 | 0.86 | 91.8 | -0.03 |
| PHA-665752 | 477575-56-7 | free base | c-Met | 92.9 | 0.28 | 115.7 | 1.08 | 115.7 | 0.73 | 109.7 | 0.53 |
| PHA-680632 | 398493-79-3 | free base | Aurora Kinase | 71.6 | -0.63 | 54.6 | -1.14 | 65.5 | -1.40 | 53.7 | -1.24 |
| PHA-767491 | 845714-00-3 | free base | CDK | 97.6 | 0.48 | 72.8 | -0.48 | 107.9 | 0.40 | 114.4 | 0.68 |
| PHA-793887 | 718630-59-2 | free base | CDK | 67.1 | -0.82 | 91.9 | 0.21 | 63.9 | -1.47 | 18.0 | -2.37 |
| Phenacetin | 62-44-2 | free base | COX | 113.7 | 1.16 | 65.3 | -0.75 | 130.6 | 1.37 | 123.2 | 0.96 |
| Phenformin HCl | 834-28-6 | hydrochloride | AMPK | 81.7 | -0.20 | 115.5 | 1.07 | 126.1 | 1.17 | 122.1 | 0.93 |
| Phenoxybenzamine HCl | 63-92-3 | hydrochloride | Adrenergic Receptor | 109.5 | 0.98 | 115.8 | 1.08 | 118.3 | 0.84 | 120.9 | 0.89 |
| Phentolamine Mesylate | 65-28-1 | mesylate | Adrenergic Receptor | 96.3 | 0.42 | 115.9 | 1.09 | 103.0 | 0.19 | 107.0 | 0.45 |
| Phenylephrine HCl | 61-76-7 | hydrochloride | Adrenergic Receptor | 94.4 | 0.34 | 49.6 | -1.32 | 118.8 | 0.86 | 141.8 | 1.55 |
| Phenytoin | 57-41-0 | free base | Sodium Channel | 80.9 | -0.23 | 58.1 | -1.01 | 102.6 | 0.17 | 139.6 | 1.48 |
| Phenytoin sodium | 630-93-3 | sodium | Sodium Channel | 83.2 | -0.14 | 115.7 | 1.08 | 105.9 | 0.32 | 124.4 | 1.00 |
| Phosphoramidon Disodium Salt | 164204-38-0 | Salt | Others | 78.0 | -0.36 | 73.6 | -0.45 | 126.1 | 1.17 | 74.1 | -0.59 |
| PHT-427 | 1191951-57-1 | free base | PDK-1,Akt | 87.7 | 0.05 | 59.1 | -0.98 | 111.2 | 0.54 | 97.7 | 0.15 |
| PI-103 | 371935-74-9 | free base | PI3K, Autophagy, DNA-PK, mTOR | 38.9 | -2.01 | 49.0 | -1.35 | 58.0 | -1.72 | 55.3 | -1.19 |
| PI-1840 | 1401223-22-0 | free base | Proteasome | 90.2 | 0.16 | 107.1 | 0.77 | 101.3 | 0.12 | 104.2 | 0.36 |
| Piceatannol | 10083-24-6 | free base | Syk | 102.6 | 0.69 | 64.9 | -0.77 | 127.2 | 1.22 | 120.4 | 0.87 |
| Pifithrin-α (PFTα) | 63208-82-2 | HBr | p53, Autophagy | 100.5 | 0.60 | 77.2 | -0.32 | 107.4 | 0.38 | 110.0 | 0.54 |
| Pifithrin-μ | 64984-31-2 | free base | p53 | 106.0 | 0.83 | 74.3 | -0.43 | 128.3 | 1.27 | 108.0 | 0.48 |
| PIK-293 | 900185-01-5 | free base | PI3K | 108.7 | 0.94 | 62.9 | -0.84 | 88.6 | -0.42 | 110.7 | 0.57 |
| PIK-294 | 900185-02-6 | free base | PI3K | 111.6 | 1.07 | 57.6 | -1.03 | 79.7 | -0.80 | 82.4 | -0.33 |
| PIK-75 | 372196-77-5 | hydrochloride | PI3K, DNA-PK | 49.3 | -1.57 | 36.8 | -1.79 | 31.7 | -2.84 | 11.9 | -2.56 |
| PIK-93 | 593960-11-3 | free base | PI3K | 64.8 | -0.91 | 73.7 | -0.45 | 113.9 | 0.66 | 85.4 | -0.23 |
| Pimasertib (AS-703026) | 1236699-92-5 | free base | MEK | 99.7 | 0.56 | 29.6 | -2.05 | 57.1 | -1.76 | 76.3 | -0.52 |
| Pimobendan | 74150-27-9 | free base | PDE | 77.7 | -0.37 | 113.1 | 0.99 | 105.7 | 0.31 | 79.0 | -0.44 |

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|---------------------------------|--------------|---------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Pioglitazone HCl | 112529-15-4 | hydrochloride | P450 (e.g. CYP17) | 100.3 | 0.59 | 116.9 | 1.12 | 99.9 | 0.06 | 123.1 | 0.96 |
| Pirarubicin | 72496-41-4 | free base | Topoisomerase | 8.8 | -3.29 | 48.7 | -1.35 | 71.3 | -1.15 | 4.4 | -2.80 |
| Pirfenidone | 53179-13-8 | free base | TGF-beta/Smad | 82.9 | -0.15 | 53.4 | -1.18 | 100.2 | 0.07 | 109.0 | 0.51 |
| Piroxicam | 36322-90-4 | free base | COX | 107.7 | 0.90 | 114.1 | 1.02 | 108.3 | 0.42 | 73.1 | -0.62 |
| PJ34 | 344458-19-1 | hydrochloride | PARP | 81.9 | -0.19 | 63.5 | -0.82 | 101.6 | 0.13 | 83.3 | -0.30 |
| PJ34 HCl | 344458-15-7 | Salt | PARP | 77.9 | -0.36 | 67.5 | -0.67 | 93.3 | -0.22 | 119.9 | 0.86 |
| PluriSIn #1 (NSC 14613) | 91396-88-2 | free base | Dehydrogenase | 73.1 | -0.56 | 112.1 | 0.95 | 94.7 | -0.16 | 134.5 | 1.32 |
| PLX-4720 | 918505-84-7 | free base | Raf | 121.0 | 1.46 | 116.8 | 1.12 | 190.3 | 3.90 | 69.4 | -0.74 |
| PNU-120596 | 501925-31-1 | free base | AChR | 75.6 | -0.46 | 112.2 | 0.95 | 99.9 | 0.06 | 127.9 | 1.11 |
| Pomalidomide | 19171-19-8 | free base | TNF-alpha | 86.4 | 0.00 | 114.3 | 1.03 | 111.2 | 0.54 | 93.5 | 0.02 |
| Ponatinib (AP24534) | 943319-70-8 | free base | PDGFR,FGFR,VEGFR,Bcr-Abl | 73.9 | -0.53 | 102.0 | 0.58 | 72.5 | -1.10 | 52.8 | -1.27 |
| PP1 | 172889-26-8 | free base | Src | 77.0 | -0.40 | 116.4 | 1.11 | 105.4 | 0.30 | 84.3 | -0.27 |
| PP121 | 1092788-83-4 | free base | DNA-PK,PDGFR,mTOR | 60.4 | -1.10 | 52.6 | -1.21 | 126.3 | 1.18 | 72.9 | -0.63 |
| PP2 | 172889-27-9 | free base | Src | 98.5 | 0.51 | 116.7 | 1.11 | 83.3 | -0.65 | 119.0 | 0.83 |
| PP242 | 1092351-67-1 | free base | mTOR,Autophagy | 70.9 | -0.66 | 50.6 | -1.29 | 79.4 | -0.81 | 63.2 | -0.94 |
| PQ 401 | 196868-63-0 | free base | IGF-1R | 71.8 | -0.62 | 56.8 | -1.06 | 102.2 | 0.16 | 105.7 | 0.41 |
| PR-619 | 2645-32-1 | free base | DUB | 67.4 | -0.80 | 53.7 | -1.17 | | | 88.1 | -0.15 |
| Pracinostat (SB939) | 929016-96-6 | free base | HDAC | 11.1 | -3.19 | 49.3 | -1.33 | 53.2 | -1.92 | 3.5 | -2.83 |
| Pralatrexate | 146464-95-1 | free base | DHFR | 116.2 | 1.26 | 91.5 | 0.20 | 93.6 | -0.21 | 70.1 | -0.72 |
| Pramipexole | 104632-26-0 | free base | Dopamine Receptor | 111.0 | 1.04 | 83.9 | -0.08 | 118.2 | 0.84 | 109.4 | 0.52 |
| Prasugrel | 150322-43-3 | free base | P2 Receptor | 95.7 | 0.39 | 112.1 | 0.95 | 127.3 | 1.23 | 105.0 | 0.39 |
| Pravastatin sodium | 81131-70-6 | free base | HMG-CoA Reductase | 117.3 | 1.31 | 113.2 | 0.99 | 113.8 | 0.65 | 129.8 | 1.17 |
| Pregnenolone | 145-13-1 | free base | Estrogen/progestogen Receptor | 128.2 | 1.77 | 114.0 | 1.02 | 111.2 | 0.54 | 127.3 | 1.09 |
| Pritelivir (BAY 57-1293) | 348086-71-5 | free base | Others | 87.5 | 0.05 | 57.3 | -1.04 | 101.3 | 0.12 | 85.0 | -0.25 |
| Procainamide HCl | 614-39-1 | Salt | Sodium Channel | 87.1 | 0.03 | 84.8 | -0.04 | 84.0 | -0.62 | 110.9 | 0.57 |
| Procaine HCl | 51-05-8 | hydrochloride | Sodium Channel | 96.9 | 0.44 | 85.5 | -0.02 | 108.3 | 0.42 | 125.1 | 1.02 |
| Promethazine HCl | 58-33-3 | Salt | Histamine Receptor | 93.1 | 0.28 | 73.9 | -0.44 | 86.7 | -0.50 | 105.8 | 0.41 |
| Propafenone HCl | 34183-22-7 | free base | Sodium Channel | 89.8 | 0.14 | 117.4 | 1.14 | 112.1 | 0.58 | 105.2 | 0.39 |

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| Proparacaine HCl | 5875-06-9 | hydrochloride | Sodium Channel | 98.3 | 0.50 | 115.3 | 1.06 | 116.0 | 0.75 | 93.6 | 0.03 |
| Propranolol HCl | 318-98-9 | hydrochloride | Adrenergic Receptor | 139.4 | 2.25 | 113.9 | 1.01 | 98.1 | -0.02 | 110.4 | 0.56 |
| PRT062607 (P505-15, BIIB057) HCl | 1370261-97-4 | hydrochloride | Syk | 65.4 | -0.89 | 61.7 | -0.88 | 105.2 | 0.28 | 85.6 | -0.23 |
| Prucalopride | 179474-81-8 | free base | 5-HT Receptor | 101.9 | 0.66 | 81.6 | -0.16 | 103.7 | 0.22 | 100.4 | 0.24 |
| PRX-08066 Maleic acid | 866206-55-5 | maleate | 5-HT Receptor | 92.5 | 0.26 | 65.3 | -0.75 | 106.3 | 0.33 | 78.6 | -0.45 |
| PTC-209 | 315704-66-6 | free base | BMI | 27.3 | -2.50 | 94.5 | 0.31 | 84.0 | -0.61 | 37.6 | -1.75 |
| PTC-209 HBr | 1217022-63-3 | free base | Others | 25.0 | -2.60 | 50.7 | -1.28 | 105.1 | 0.28 | 37.1 | -1.76 |
| PU-H71 | 873436-91-0 | free base | HSP (e.g. HSP90) | 41.3 | -1.91 | 42.7 | -1.57 | 41.3 | -2.43 | 50.5 | -1.34 |
| Purmorphamine | 483367-10-8 | free base | Hedgehog/Smoothened | 104.3 | 0.76 | 66.2 | -0.72 | 113.9 | 0.65 | 123.4 | 0.97 |
| Puromycin 2HCl | 58-58-2 | Salt | Others | 15.3 | -3.01 | 74.1 | -0.43 | 63.2 | -1.50 | 1.4 | -2.90 |
| PYR-41 | 418805-02-4 | free base | E1 Activating | 68.7 | -0.75 | 60.2 | -0.94 | | | 139.4 | 1.48 |
| Pyridostigmine Bromide | 101-26-8 | bromide | AChR | 126.4 | 1.69 | 110.3 | 0.88 | 114.6 | 0.68 | 95.7 | 0.09 |
| Pyrimethamine | 58-14-0 | free base | DHFR | 95.7 | 0.39 | 116.5 | 1.11 | 107.1 | 0.37 | 129.5 | 1.16 |
| QNZ (EVP4593) | 545380-34-5 | free base | TNF-alpha,NF-kB | 57.3 | -1.23 | 49.0 | -1.34 | 95.3 | -0.13 | 82.6 | -0.32 |
| Quercetin | 117-39-5 | free base | PKC,Src,PI3K,Sirtuin | 130.6 | 1.87 | 99.3 | 0.48 | 85.8 | -0.54 | 80.4 | -0.39 |
| Quetiapine Fumarate | 111974-72-2 | fumarate | Dopamine Receptor | 113.6 | 1.15 | 114.0 | 1.02 | 108.9 | 0.44 | 115.2 | 0.71 |
| Quinapril HCl | 82586-55-8 | hydrochloride | RAAS | 94.5 | 0.34 | 56.2 | -1.08 | 129.1 | 1.30 | 110.4 | 0.56 |
| Quisinostat (JNJ-26481585) | 875320-29-9 | free base | HDAC | 20.3 | -2.80 | 20.6 | -2.38 | 16.4 | -3.49 | 2.5 | -2.86 |
| Quizartinib (AC220) | 950769-58-1 | free base | FLT3 | 77.3 | -0.38 | 93.8 | 0.28 | 109.6 | 0.47 | 87.1 | -0.18 |
| R406 | 841290-81-1 | besylate | Syk,FLT3 | 89.3 | 0.12 | 112.9 | 0.98 | 86.8 | -0.50 | 78.6 | -0.45 |
| R406 (free base) | 841290-80-0 | free base | Syk | 87.3 | 0.04 | 114.5 | 1.03 | 106.4 | 0.34 | 86.1 | -0.21 |
| R547 | 741713-40-6 | free base | CDK | 56.2 | -1.28 | 81.1 | -0.18 | 58.0 | -1.72 | 28.5 | -2.04 |
| Racecadotril | 81110-73-8 | free base | Opioid Receptor | 88.6 | 0.09 | 56.2 | -1.08 | 145.5 | 2.00 | 99.0 | 0.20 |
| RAF265 (CHIR-265) | 927880-90-8 | free base | VEGFR,Raf | 92.4 | 0.25 | 59.4 | -0.97 | 82.6 | -0.67 | 59.0 | -1.07 |
| Raloxifene HCl | 82640-04-8 | hydrochloride | Estrogen/progestogen Receptor | 102.4 | 0.68 | 109.4 | 0.85 | 127.7 | 1.24 | 73.0 | -0.63 |
| Raltegravir (MK-0518) | 518048-05-0 | free base | Integrase | 96.4 | 0.42 | 54.2 | -1.16 | 118.0 | 0.83 | 151.5 | 1.86 |
| Ramelteon | 196597-26-9 | free base | MT Receptor | 111.3 | 1.05 | 94.3 | 0.30 | 110.3 | 0.50 | 95.5 | 0.09 |
| Ramipril | 87333-19-5 | free base | RAAS | 104.7 | 0.78 | 117.1 | 1.13 | 103.2 | 0.20 | 96.9 | 0.13 |

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|---|--------------|-----------------|-----------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ranitidine | 66357-59-3 | hydrochloride | Histamine Receptor | 105.3 | 0.80 | 116.5 | 1.11 | 108.1 | 0.41 | 97.1 | 0.14 |
| Ranolazine 2HCl | 95635-56-6 | dihydrochloride | Calcium Channel | 80.2 | -0.26 | 78.0 | -0.29 | 102.1 | 0.15 | 98.4 | 0.18 |
| Rapamycin (Sirolimus) | 53123-88-9 | free base | Autophagy,mTOR | 70.9 | -0.66 | 59.4 | -0.97 | 51.7 | -1.99 | 81.0 | -0.37 |
| Rasagiline Mesylate | 161735-79-1 | mesylate | MAO | 96.9 | 0.44 | 116.1 | 1.09 | 93.5 | -0.21 | 130.0 | 1.18 |
| Refametinib (RDEA119, Bay 86-9766) | 923032-37-5 | free base | MEK | | | 33.3 | -1.92 | 38.4 | -2.55 | 104.2 | 0.36 |
| Regorafenib (BAY 73-4506) | 755037-03-7 | free base | c-RET,VEGFR | 93.4 | 0.30 | 79.8 | -0.22 | 61.4 | -1.57 | 66.4 | -0.84 |
| Repaglinide | 135062-02-1 | free base | Potassium Channel | 76.7 | -0.41 | 71.6 | -0.52 | 86.1 | -0.53 | 93.0 | 0.01 |
| RepSox | 446859-33-2 | free base | TGF-beta/Smad | 78.1 | -0.35 | 54.5 | -1.14 | | | 104.1 | 0.36 |
| Resminostat | 864814-88-0 | free base | HDAC | 56.4 | -1.27 | 112.6 | 0.97 | 128.5 | 1.28 | 35.7 | -1.81 |
| Resveratrol | 501-36-0 | free base | Sirtuin,Autophagy | 78.3 | -0.34 | 115.4 | 1.07 | 100.1 | 0.07 | 97.5 | 0.15 |
| RG108 | 48208-26-0 | free base | Transferase,DNA Methyltransferase | 91.1 | 0.20 | 59.6 | -0.96 | 83.0 | -0.66 | 112.4 | 0.62 |
| RG2833 (RGFP109) | 1215493-56-3 | free base | HDAC | 75.8 | -0.45 | 101.3 | 0.56 | 129.3 | 1.31 | 98.0 | 0.17 |
| RGFP966 | 1396841-57-8 | free base | HDAC | 91.0 | 0.19 | 93.3 | 0.27 | | | 120.4 | 0.87 |
| Ridaforolimus (Deforolimus, MK-8669) | 572924-54-0 | free base | mTOR | 66.0 | -0.86 | 67.5 | -0.67 | 72.7 | -1.09 | 63.4 | -0.93 |
| Rigosertib (ON-01910) | 1225497-78-8 | sodium | PLK | 83.1 | -0.14 | 52.7 | -1.21 | 123.5 | 1.06 | 90.7 | -0.07 |
| Rilpivirine | 500287-72-9 | free base | Reverse Transcriptase | 73.5 | -0.55 | 82.7 | -0.12 | 72.7 | -1.10 | 71.1 | -0.69 |
| Riluzole | 1744-22-5 | free base | Sodium Channel | 88.8 | 0.10 | 114.4 | 1.03 | 101.8 | 0.14 | 89.0 | -0.12 |
| Rimonabant | 168273-06-1 | free base | Cannabinoid Receptor | 135.9 | 2.10 | 109.1 | 0.84 | 117.0 | 0.79 | 93.2 | 0.01 |
| Risperidone | 106266-06-2 | free base | 5-HT Receptor | 82.3 | -0.17 | 114.2 | 1.03 | 104.3 | 0.25 | 77.7 | -0.48 |
| RITA (NSC 652287) | 213261-59-7 | free base | E3 Ligase ,p53 | 88.5 | 0.09 | 83.6 | -0.09 | 127.7 | 1.24 | 52.3 | -1.28 |
| Ritodrine HCl | 23239-51-2 | hydrochloride | Adrenergic Receptor | 92.7 | 0.27 | 115.9 | 1.09 | 113.8 | 0.65 | 122.1 | 0.93 |
| Ritonavir | 155213-67-5 | free base | HIV Protease | 117.1 | 1.30 | 116.3 | 1.10 | 122.6 | 1.02 | 68.0 | -0.79 |
| Rivaroxaban | 366789-02-8 | free base | Factor Xa | 139.0 | 2.23 | 107.3 | 0.77 | 109.1 | 0.45 | 113.3 | 0.65 |
| Rivastigmine Tartrate | 129101-54-8 | tartrate | AChR | 96.4 | 0.42 | 116.3 | 1.10 | 75.1 | -0.99 | 126.2 | 1.06 |
| Rizatriptan Benzoate | 145202-66-0 | benzoate | 5-HT Receptor | 110.7 | 1.03 | 114.7 | 1.04 | 106.7 | 0.35 | 91.7 | -0.03 |
| RKI-1447 | 1342278-01-6 | free base | ROCK | 70.9 | -0.65 | 86.1 | 0.00 | | | 124.5 | 1.00 |
| Ro 31-8220 Mesylate | 138489-18-6 | mesylate | PKC | 49.6 | -1.56 | 74.8 | -0.41 | | | 40.4 | -1.66 |
| Ro3280 | 1062243-51-9 | free base | PLK | 54.0 | -1.37 | 58.6 | -1.00 | | | 25.0 | -2.15 |

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|--|--------------|---------------|--------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| RO4929097 | 847925-91-1 | free base | Gamma-secretase | 106.8 | 0.86 | 115.0 | 1.05 | 101.6 | 0.13 | 76.1 | -0.53 |
| Rocilinostat (ACY-1215) | 1316214-52-4 | free base | HDAC | 76.6 | -0.41 | 67.6 | -0.67 | 122.9 | 1.04 | 111.6 | 0.59 |
| Rocuronium Bromide | 119302-91-9 | bromide | AChR | 74.2 | -0.52 | 115.8 | 1.08 | 91.2 | -0.31 | 84.5 | -0.26 |
| Rofecoxib | 162011-90-7 | free base | COX | 97.4 | 0.47 | 120.1 | 1.24 | 108.1 | 0.41 | 116.0 | 0.74 |
| Roflumilast | 162401-32-3 | free base | PDE | 125.2 | 1.64 | 99.4 | 0.49 | 96.9 | -0.07 | 74.7 | -0.57 |
| Rolipram | 61413-54-5 | free base | PDE | 91.9 | 0.23 | 63.3 | -0.83 | 115.0 | 0.70 | 101.5 | 0.27 |
| Roscovitine (Seliciclib,CYC202) | 186692-46-6 | free base | CDK | 95.5 | 0.39 | 110.6 | 0.90 | 111.1 | 0.54 | 63.5 | -0.93 |
| Rosiglitazone | 122320-73-4 | free base | PPAR | 79.3 | -0.30 | 72.3 | -0.50 | 104.0 | 0.23 | 117.9 | 0.80 |
| Rosuvastatin Calcium | 147098-20-2 | free base | RAAS | 89.9 | 0.15 | 74.6 | -0.42 | 91.0 | -0.32 | 96.9 | 0.13 |
| Rotigotine | 99755-59-6 | free base | Dopamine Receptor | 106.8 | 0.87 | 116.8 | 1.12 | 89.2 | -0.39 | 94.8 | 0.06 |
| Rotundine | 483-14-7 | free base | Dopamine Receptor | 107.9 | 0.91 | 111.0 | 0.91 | 80.7 | -0.75 | 111.8 | 0.60 |
| Roxatidine Acetate HCl | 93793-83-0 | hydrochloride | Histamine Receptor | 97.3 | 0.46 | 115.7 | 1.08 | 118.3 | 0.84 | 160.5 | 2.14 |
| RS-127445 | 199864-87-3 | free base | 5-HT Receptor | 75.6 | -0.46 | 47.6 | -1.40 | 114.2 | 0.67 | 137.9 | 1.43 |
| Rucaparib (AG-014699,PF-01367338) | 459868-92-9 | phosphate | PARP | | | 79.5 | -0.24 | 74.0 | -1.04 | 99.5 | 0.21 |
| Rufinamide | 106308-44-5 | free base | Sodium Channel | 99.0 | 0.53 | 81.0 | -0.18 | 83.3 | -0.64 | 90.9 | -0.06 |
| Rupatadine Fumarate | 182349-12-8 | fumarate | Histamine Receptor | 116.7 | 1.28 | 103.1 | 0.62 | 113.4 | 0.64 | 130.4 | 1.19 |
| Ruxolitinib (INCB018424) | 941678-49-5 | free base | JAK | 99.4 | 0.55 | 115.0 | 1.05 | 105.6 | 0.30 | 109.6 | 0.53 |
| RVX-208 | 1044870-39-4 | free base | Epigenetic Reader Domain | 134.1 | 2.02 | 93.5 | 0.27 | 100.4 | 0.08 | 88.3 | -0.14 |
| S- (+)-Rolipram | 85416-73-5 | free base | PDE | 121.6 | 1.49 | 96.0 | 0.36 | 92.2 | -0.27 | 81.7 | -0.35 |
| S3I-201 | 501919-59-1 | free base | STAT | 98.3 | 0.50 | 84.7 | -0.05 | 119.5 | 0.89 | 85.9 | -0.22 |
| Sabutoclax | 1228108-65-3 | free base | Bcl-2 | 85.2 | -0.05 | 88.6 | 0.09 | 100.8 | 0.10 | 72.1 | -0.65 |
| Safinamide Mesylate | 202825-46-5 | mesylate | MAO | 110.9 | 1.04 | 112.4 | 0.96 | 107.0 | 0.36 | 68.0 | -0.79 |
| Sal003 | 1164470-53-4 | free base | ELF2 | 132.8 | 1.96 | 99.5 | 0.49 | 102.3 | 0.16 | 107.5 | 0.47 |
| SANT-1 | 304909-07-7 | free base | Hedgehog/Smoothened | 93.8 | 0.31 | 105.1 | 0.69 | | | 90.9 | -0.06 |
| Santacruzamate A (CAY10683) | 1477949-42-0 | free base | HDAC | 60.3 | -1.11 | 91.7 | 0.21 | 82.0 | -0.70 | 75.8 | -0.54 |
| SAR131675 | 1433953-83-3 | free base | VEGFR | 81.0 | -0.23 | 121.6 | 1.29 | 116.0 | 0.74 | 114.4 | 0.68 |
| SAR245409 (XL765) | 1349796-36-6 | free base | PI3K,mTOR | 89.7 | 0.14 | 56.2 | -1.08 | 111.1 | 0.54 | 97.1 | 0.13 |
| Saracatinib (AZD0530) | 379231-04-6 | free base | Src,Bcr-Abl | 113.4 | 1.14 | 111.0 | 0.91 | 91.9 | -0.28 | 108.9 | 0.51 |
| Saxagliptin | 361442-04-8 | free base | DPP-4 | 92.3 | 0.25 | 115.5 | 1.07 | 106.3 | 0.33 | 99.2 | 0.20 |

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|--------------------------------|--------------|---------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| SB202190 (FHPI) | 152121-30-7 | free base | p38 MAPK | | | 72.0 | -0.51 | 92.1 | -0.27 | 79.0 | -0.44 |
| SB203580 | 152121-47-6 | free base | p38 MAPK | 78.1 | -0.35 | 111.3 | 0.92 | 118.3 | 0.84 | 78.0 | -0.47 |
| SB216763 | 280744-09-4 | free base | GSK-3 | 92.3 | 0.25 | 113.2 | 0.99 | 93.0 | -0.23 | 85.1 | -0.25 |
| SB269970 HCl | 261901-57-9 | hydrochloride | 5-HT Receptor | 74.4 | -0.51 | 115.0 | 1.05 | 117.6 | 0.81 | 109.2 | 0.52 |
| SB271046 | 209481-20-9 | free base | 5-HT Receptor | 93.6 | 0.30 | 114.9 | 1.05 | 90.9 | -0.32 | 127.7 | 1.11 |
| SB-3CT | 292605-14-2 | free base | MMP | 82.8 | -0.15 | 77.2 | -0.32 | 93.4 | -0.22 | 72.6 | -0.64 |
| SB408124 | 288150-92-5 | free base | OX Receptor | 119.2 | 1.39 | 56.8 | -1.06 | 109.6 | 0.47 | 96.3 | 0.11 |
| SB415286 | 264218-23-7 | free base | GSK-3 | 87.3 | 0.04 | 113.2 | 0.99 | 113.1 | 0.62 | 123.9 | 0.98 |
| SB431542 | 301836-41-9 | free base | TGF-beta/Smad | 87.8 | 0.06 | 91.6 | 0.20 | 84.5 | -0.59 | 107.0 | 0.45 |
| SB505124 | 694433-59-5 | free base | TGF-beta/Smad | 102.6 | 0.69 | 59.5 | -0.96 | 95.1 | -0.14 | 92.9 | 0.00 |
| SB525334 | 356559-20-1 | free base | TGF-beta/Smad | 101.4 | 0.64 | 105.6 | 0.71 | 116.6 | 0.77 | 75.6 | -0.55 |
| SB590885 | 405554-55-4 | free base | Raf | 122.0 | 1.51 | 74.4 | -0.42 | 108.6 | 0.43 | 131.4 | 1.22 |
| SB705498 | 501951-42-4 | free base | TRPV | 76.1 | -0.44 | 111.6 | 0.93 | 106.7 | 0.35 | 98.3 | 0.17 |
| SB742457 | 607742-69-8 | free base | 5-HT Receptor | 90.1 | 0.15 | 78.7 | -0.27 | 126.8 | 1.20 | 111.8 | 0.60 |
| SB743921 | 940929-33-9 | hydrochloride | Kinesin | 72.4 | -0.59 | 54.8 | -1.14 | 41.3 | -2.43 | 55.5 | -1.18 |
| SC-514 | 354812-17-2 | free base | IκB/IKK | 87.0 | 0.03 | 69.4 | -0.60 | 84.2 | -0.61 | 109.8 | 0.54 |
| SC75741 | 913822-46-5 | free base | NF-κB | 67.6 | -0.80 | 74.9 | -0.40 | 110.1 | 0.50 | 71.1 | -0.69 |
| Scopine | 498-45-3 | free base | Adrenergic Receptor | 81.2 | -0.22 | 116.7 | 1.12 | 120.5 | 0.94 | 147.5 | 1.73 |
| Scopolamine HBr | 114-49-8 | hydrobromide | AChR | 79.9 | -0.28 | 116.6 | 1.11 | 123.3 | 1.05 | 97.7 | 0.15 |
| Scriptaid | 287383-59-9 | free base | HDAC | 71.5 | -0.63 | 64.7 | -0.77 | 102.2 | 0.16 | 53.7 | -1.24 |
| Selumetinib (AZD6244) | 606143-52-6 | free base | MEK | 121.5 | 1.48 | 106.5 | 0.75 | 48.4 | -2.13 | 83.0 | -0.31 |
| Semagacestat (LY450139) | 425386-60-3 | free base | Gamma-secretase | 87.0 | 0.03 | 115.7 | 1.08 | 122.4 | 1.01 | 92.4 | -0.01 |
| Semaxanib (SU5416) | 194413-58-6 | free base | VEGFR | 83.4 | -0.13 | 54.5 | -1.15 | 119.4 | 0.89 | 100.8 | 0.25 |
| Sertraline HCl | 79559-97-0 | hydrochloride | 5-HT Receptor | 106.9 | 0.87 | 59.7 | -0.96 | 98.3 | -0.01 | 128.2 | 1.12 |
| SF1670 | 345630-40-2 | free base | Others | 82.6 | -0.16 | 90.3 | 0.16 | 114.3 | 0.67 | 95.1 | 0.07 |
| SGC 0946 | N/A | free base | Histone Methyltransferase | 91.6 | 0.22 | 88.0 | 0.07 | 90.6 | -0.33 | 110.4 | 0.56 |
| SGC-CBP30 | N/A | free base | Epigenetic Reader Domain | 75.5 | -0.46 | 101.2 | 0.55 | | | 104.1 | 0.36 |
| SGI-1027 | 1020149-73-8 | free base | DNA Methyltransferase | 81.2 | -0.22 | 98.0 | 0.44 | 103.1 | 0.20 | 5.1 | -2.78 |
| SGI-1776 free base | 1025065-69-3 | free base | Pim | 83.5 | -0.12 | 75.3 | -0.39 | 83.7 | -0.63 | 93.1 | 0.01 |

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|--|--------------|---------------|--------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| SGX-523 | 1022150-57-7 | free base | c-Met | 107.2 | 0.88 | 100.8 | 0.54 | 74.8 | -1.01 | 96.2 | 0.11 |
| SH-4-54 | 1456632-40-8 | free base | STAT | 81.6 | -0.20 | 57.0 | -1.05 | 104.9 | 0.27 | 99.1 | 0.20 |
| Sildenafil Citrate | 171599-83-0 | citrate | PDE | 102.1 | 0.66 | 115.8 | 1.08 | 101.5 | 0.13 | 83.6 | -0.29 |
| Silodosin | 160970-54-7 | free base | Adrenergic Receptor | 84.5 | -0.08 | 114.0 | 1.02 | 113.5 | 0.64 | 96.6 | 0.12 |
| Sirtinol | 410536-97-9 | free base | Sirtuin | 88.1 | 0.07 | 114.6 | 1.04 | 110.0 | 0.49 | 80.5 | -0.39 |
| Sitagliptin phosphate monohydrate | 654671-77-9 | phosphate | DPP-4 | 93.4 | 0.30 | 94.3 | 0.30 | 100.6 | 0.09 | 117.9 | 0.80 |
| Sitaxentan sodium | 210421-74-2 | free base | Endothelin Receptor | 99.6 | 0.56 | 89.2 | 0.12 | 113.8 | 0.65 | 96.0 | 0.10 |
| Skepinone-L | 1221485-83-1 | free base | p38 MAPK | 66.3 | -0.85 | 52.3 | -1.22 | | | 94.0 | 0.04 |
| SKI II | 312636-16-1 | free base | S1P Receptor | 80.8 | -0.24 | 56.0 | -1.09 | | | 126.9 | 1.08 |
| SKLB1002 | 1225451-84-2 | free base | VEGFR | 84.4 | -0.08 | 57.3 | -1.04 | | | 103.9 | 0.35 |
| SL-327 | 305350-87-2 | free base | MEK | 75.2 | -0.47 | 104.4 | 0.67 | 94.9 | -0.15 | 108.2 | 0.49 |
| SMI-4a | 438190-29-5 | free base | Pim | 76.0 | -0.44 | 72.1 | -0.51 | 101.5 | 0.13 | 84.0 | -0.28 |
| SN-38 | 86639-52-3 | free base | Topoisomerase | 3.5 | -3.51 | 32.3 | -1.95 | 61.7 | -1.56 | 4.2 | -2.81 |
| SNS-032 (BMS-387032) | 345627-80-7 | free base | CDK | 52.6 | -1.43 | 36.6 | -1.80 | 27.8 | -3.00 | 11.0 | -2.59 |
| SNS-314 Mesylate | 1146618-41-8 | mesylate | Aurora Kinase | 58.0 | -1.20 | 65.3 | -0.75 | 75.0 | -1.00 | 69.9 | -0.73 |
| SNX-2112 (PF-04928473) | 908112-43-6 | free base | HSP (e.g. HSP90) | 51.3 | -1.49 | 36.8 | -1.79 | 40.4 | -2.47 | 50.2 | -1.35 |
| Sodium 4-Aminosalicylate | 6018-19-5 | sodium | NF-kB | 96.3 | 0.42 | 118.5 | 1.18 | 106.0 | 0.32 | 132.6 | 1.26 |
| Sodium Danshensu | 67920-52-9 | sodium | Others,P450 (e.g. CYP17) | 110.0 | 1.00 | 77.4 | -0.31 | 105.2 | 0.29 | 106.8 | 0.44 |
| Sodium Phenylbutyrate | 1716-12-7 | free base | HDAC | 91.7 | 0.22 | 98.2 | 0.44 | 83.7 | -0.63 | 89.1 | -0.12 |
| Sofosbuvir (PSI-7977, GS-7977) | 1190307-88-0 | free base | DNA/RNA Synthesis | 104.2 | 0.75 | 104.5 | 0.67 | 101.8 | 0.14 | 90.5 | -0.07 |
| Solifenacin succinate | 242478-38-2 | succinate | AChR | 81.4 | -0.21 | 80.7 | -0.19 | 113.0 | 0.62 | 89.4 | -0.11 |
| Sorafenib | 284461-73-0 | free base | Raf | 84.4 | -0.09 | 116.2 | 1.10 | 74.5 | -1.02 | 97.2 | 0.14 |
| Sorafenib Tosylate | 475207-59-1 | tosylate | PDGFR,Raf,VEGFR | 97.8 | 0.48 | 113.7 | 1.01 | 77.3 | -0.90 | 91.1 | -0.05 |
| Sotalol | 959-24-0 | hydrochloride | Adrenergic Receptor | 89.0 | 0.11 | 116.2 | 1.10 | 125.1 | 1.13 | 137.5 | 1.41 |
| Sotrastaurin | 425637-18-9 | free base | PKC | 87.2 | 0.03 | 104.1 | 0.66 | 92.7 | -0.25 | 72.7 | -0.64 |
| SP600125 | 129-56-6 | free base | JNK | 86.8 | 0.02 | 115.0 | 1.05 | 100.0 | 0.07 | 94.0 | 0.04 |
| Spironolactone | 52-01-7 | free base | Androgen Receptor | 95.1 | 0.37 | 57.3 | -1.04 | 99.1 | 0.03 | 122.7 | 0.95 |
| SRT1720 | 1001645-58-4 | hydrochloride | Sirtuin | 89.4 | 0.13 | 113.2 | 0.99 | 86.0 | -0.53 | 62.1 | -0.97 |
| S-Ruxolitinib (INCB018424) | 941685-37-6 | free base | JAK | 74.3 | -0.51 | 54.9 | -1.13 | 83.6 | -0.63 | 99.7 | 0.22 |

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|------------------------------|--------------|---------------|--|-------|-------|-------|-------|-------|-------|-------|-------|
| SSR128129E | 848318-25-2 | free base | FGFR | 71.2 | -0.64 | 61.8 | -0.88 | | | 113.0 | 0.64 |
| Stattic | 19983-44-9 | free base | STAT | 92.2 | 0.24 | 117.1 | 1.13 | 83.4 | -0.64 | 93.0 | 0.01 |
| Stavudine (d4T) | 3056-17-5 | free base | Reverse Transcriptase | 88.9 | 0.10 | 49.7 | -1.32 | 106.8 | 0.35 | 78.5 | -0.45 |
| SU11274 | 658084-23-2 | free base | c-Met | 80.1 | -0.27 | 92.9 | 0.25 | 71.8 | -1.13 | 127.0 | 1.08 |
| Sulfacetamide Sodium | 127-56-0 | sodium | Autophagy | 103.6 | 0.73 | 116.1 | 1.09 | 109.1 | 0.45 | 97.7 | 0.16 |
| Sumatriptan Succinate | 103628-48-4 | succinate | 5-HT Receptor | 91.5 | 0.22 | 99.6 | 0.49 | 97.9 | -0.02 | 76.0 | -0.53 |
| Sunitinib Malate | 341031-54-7 | malate | VEGFR,PDGFR,c-Kit | 53.0 | -1.41 | 109.8 | 0.86 | 83.6 | -0.63 | 139.8 | 1.49 |
| Suvorexant (MK-4305) | 1030377-33-3 | free base | OX Receptor | 80.4 | -0.25 | 117.0 | 1.13 | 106.8 | 0.35 | 101.4 | 0.27 |
| Synephrine | 94-07-5 | free base | Adrenergic Receptor | 93.3 | 0.29 | 80.2 | -0.21 | 91.7 | -0.29 | 124.8 | 1.01 |
| Synephrine HCl | 5985-28-4 | hydrochloride | Adrenergic Receptor | 108.9 | 0.95 | 68.8 | -0.63 | 77.8 | -0.88 | 111.6 | 0.60 |
| T0070907 | 313516-66-4 | free base | PPAR | 88.9 | 0.10 | 100.1 | 0.51 | 125.5 | 1.15 | 116.8 | 0.76 |
| T0901317 | 293754-55-9 | free base | Liver X Receptor | 98.1 | 0.50 | 62.6 | -0.85 | 88.4 | -0.43 | 120.2 | 0.87 |
| Tadalafil | 171596-29-5 | free base | PDE | 94.7 | 0.35 | 115.7 | 1.08 | 110.3 | 0.50 | 98.1 | 0.17 |
| TAE226 (NVP-TAE226) | 761437-28-9 | free base | FAK | 32.9 | -2.27 | 38.0 | -1.74 | 61.9 | -1.55 | 77.6 | -0.48 |
| TAK-285 | 871026-44-7 | free base | EGFR,HER2 | 106.7 | 0.86 | 72.8 | -0.48 | 118.5 | 0.85 | 107.9 | 0.48 |
| TAK-438 | 1260141-27-2 | fumarate | Potassium Channel | 66.9 | -0.83 | 71.5 | -0.53 | 107.4 | 0.38 | 111.4 | 0.59 |
| TAK-632 | 1228591-30-7 | free base | Raf | 81.3 | -0.22 | 98.2 | 0.44 | 60.4 | -1.62 | 108.5 | 0.50 |
| TAK-700 (Orteronel) | 426219-18-3 | free base | P450 (e.g. CYP17) | 97.5 | 0.47 | 103.2 | 0.62 | 111.0 | 0.53 | 67.4 | -0.80 |
| TAK-715 | 303162-79-0 | free base | p38 MAPK | 80.6 | -0.25 | 112.9 | 0.98 | 92.1 | -0.27 | 93.7 | 0.03 |
| TAK-733 | 1035555-63-5 | free base | MEK | 86.1 | -0.01 | 22.8 | -2.30 | 65.8 | -1.39 | 87.2 | -0.18 |
| TAK-875 | 1374598-80-7 | hydrate | GPR | 89.1 | 0.11 | 113.5 | 1.00 | 104.5 | 0.26 | 116.7 | 0.76 |
| TAK-901 | 934541-31-8 | free base | Aurora Kinase | 40.8 | -1.93 | 86.4 | 0.01 | 43.3 | -2.34 | 50.8 | -1.33 |
| TAME | 901-47-3 | free base | E3 Ligase ,APC | 111.1 | 1.05 | 66.3 | -0.72 | 86.0 | -0.53 | 128.7 | 1.14 |
| Tamoxifen Citrate | 54965-24-1 | citrate | Estrogen/progestogen Receptor, Autophagy | 98.8 | 0.53 | 100.5 | 0.53 | 128.9 | 1.29 | 165.6 | 2.31 |
| Tandutinib (MLN518) | 387867-13-2 | free base | FLT3 | 79.0 | -0.31 | 87.5 | 0.05 | 120.0 | 0.92 | 97.1 | 0.14 |
| TAPI-1 | 171235-71-5 | free base | Others | 79.1 | -0.31 | 77.7 | -0.30 | 99.1 | 0.03 | 122.0 | 0.93 |
| Tarividar | 206873-63-4 | free base | P-gp | 64.1 | -0.94 | 61.1 | -0.91 | 96.7 | -0.07 | 110.7 | 0.57 |
| Tasisulam | 519055-62-0 | free base | Caspase | 75.1 | -0.48 | 93.8 | 0.28 | 96.9 | -0.07 | 73.6 | -0.61 |

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|---|---------------|---------------|-----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| TCID | 30675-13-9 | free base | DUB | 79.2 | -0.30 | 93.9 | 0.29 | | | 110.8 | 0.57 |
| TCS 359 | 301305-73-7 | free base | FLT3 | 98.8 | 0.53 | 68.7 | -0.63 | 109.3 | 0.46 | 81.1 | -0.37 |
| Telaprevir (VX-950) | 402957-28-2 | free base | HCV Protease | 112.4 | 1.10 | 115.5 | 1.07 | 111.4 | 0.55 | 87.0 | -0.19 |
| Telatinib | 332012-40-5 | free base | VEGFR,PDGFR,c-Kit | 109.0 | 0.96 | 61.4 | -0.90 | 98.2 | -0.01 | 107.3 | 0.46 |
| Telmisartan | 144701-48-4 | free base | RAAS | 99.5 | 0.55 | 113.2 | 0.99 | 98.0 | -0.02 | 96.2 | 0.11 |
| Telotristat Etiprate (LX 1606 Hippurate) | 11137608-69-5 | Salt | Hydroxylase | 103.8 | 0.74 | 54.5 | -1.14 | 92.1 | -0.27 | 84.7 | -0.26 |
| Temocapril HCl | 110221-44-8 | hydrochloride | RAAS | 101.8 | 0.65 | 115.7 | 1.08 | 97.8 | -0.03 | 131.0 | 1.21 |
| Temozolomide | 85622-93-1 | free base | Autophagy | 111.6 | 1.07 | 76.6 | -0.34 | 108.2 | 0.41 | 85.8 | -0.22 |
| Temsirolimus (CCI-779, NSC 683864) | 162635-04-3 | free base | mTOR | 65.6 | -0.88 | 50.8 | -1.28 | 59.6 | -1.65 | 74.3 | -0.59 |
| Tenofovir Disoproxil Fumarate | 202138-50-9 | fumarate | Reverse Transcriptase | 96.5 | 0.43 | 115.6 | 1.07 | 94.9 | -0.15 | 78.1 | -0.47 |
| Tenovin-1 | 380315-80-0 | free base | p53,E3 Ligase | 82.0 | -0.19 | 68.4 | -0.64 | 103.7 | 0.22 | 105.1 | 0.39 |
| Tenovin-6 | 1011557-82-6 | free base | p53 | 77.5 | -0.38 | 116.7 | 1.12 | 109.3 | 0.46 | 111.9 | 0.61 |
| Terazosin HCl | 70024-40-7 | hydrochloride | Adrenergic Receptor | 88.2 | 0.07 | 69.9 | -0.58 | 99.8 | 0.06 | 117.5 | 0.78 |
| Tetracaine HCl | 136-47-0 | hydrochloride | Calcium Channel | 99.2 | 0.54 | 113.9 | 1.02 | 145.3 | 1.99 | 106.4 | 0.43 |
| Tetrahydrozoline HCl | 522-48-5 | free base | Adrenergic Receptor | 92.6 | 0.26 | 105.0 | 0.69 | 106.8 | 0.35 | 92.8 | 0.00 |
| Tetrandrine | 518-34-3 | free base | Calcium Channel | 114.1 | 1.17 | 113.0 | 0.98 | 88.3 | -0.43 | 81.4 | -0.36 |
| TG003 | 300801-52-9 | free base | CDK | 71.6 | -0.63 | 117.3 | 1.14 | 92.2 | -0.27 | 67.5 | -0.80 |
| TG100-115 | 677297-51-7 | free base | PI3K | 88.2 | 0.08 | 51.3 | -1.26 | 131.6 | 1.41 | 101.6 | 0.28 |
| TG100713 | 925705-73-3 | free base | PI3K | 98.9 | 0.53 | 94.8 | 0.32 | 111.6 | 0.56 | 103.7 | 0.35 |
| TG101209 | 936091-14-4 | free base | JAK,FLT3,c-RET | 51.7 | -1.47 | 104.4 | 0.67 | 91.8 | -0.28 | 52.7 | -1.27 |
| TG101348 (SAR302503) | 936091-26-8 | free base | JAK | 42.8 | -1.85 | 112.1 | 0.95 | 86.6 | -0.50 | 54.7 | -1.21 |
| TGX-221 | 663619-89-4 | free base | PI3K | 88.6 | 0.09 | 75.1 | -0.40 | 112.3 | 0.59 | 64.6 | -0.89 |
| Thalidomide | 50-35-1 | free base | TNF-alpha,E3 Ligase | 97.4 | 0.47 | 101.7 | 0.57 | 106.0 | 0.32 | 104.7 | 0.38 |
| Thiazovivin | 1226056-71-8 | free base | ROCK | 94.6 | 0.35 | 68.1 | -0.65 | 104.6 | 0.26 | 89.3 | -0.11 |
| Tianeptine sodium | 30123-17-2 | sodium | 5-HT Receptor | 97.8 | 0.48 | 49.1 | -1.34 | 114.7 | 0.69 | 68.1 | -0.78 |
| TIC10 | 41276-02-2 | free base | Akt | 86.2 | -0.01 | 63.0 | -0.84 | | | 125.3 | 1.03 |
| Ticagrelor | 274693-27-5 | free base | P2 Receptor | 98.7 | 0.52 | 117.0 | 1.13 | 94.5 | -0.17 | 102.3 | 0.30 |
| Tie2 kinase inhibitor | 948557-43-5 | free base | Tie-2 | 111.7 | 1.07 | 82.8 | -0.12 | 118.3 | 0.84 | 93.3 | 0.02 |

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|--|--------------|---------------|-------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Timolol Maleate | 26921-17-5 | maleate | Adrenergic Receptor | 86.3 | 0.00 | 117.5 | 1.15 | 93.0 | -0.23 | 121.9 | 0.92 |
| Tiotropium Bromide hydrate | 139404-48-1 | hydrate | AChR | 81.0 | -0.23 | 57.6 | -1.03 | 118.8 | 0.86 | 124.7 | 1.01 |
| Tioxolone | 4991-65-5 | free base | Carbonic Anhydrase | 92.9 | 0.27 | 108.5 | 0.82 | 140.8 | 1.80 | 129.6 | 1.16 |
| Tipifarnib | 192185-72-1 | free base | Transferase | 70.3 | -0.68 | 106.4 | 0.74 | 65.6 | -1.40 | 53.2 | -1.26 |
| Tivozanib (AV-951) | 475108-18-0 | free base | VEGFR,PDGFR,c-Kit | 80.0 | -0.27 | 114.8 | 1.05 | 130.5 | 1.36 | 90.0 | -0.09 |
| Tizanidine HCl | 64461-82-1 | hydrochloride | Adrenergic Receptor | 112.0 | 1.08 | 56.0 | -1.09 | 130.1 | 1.34 | 79.5 | -0.42 |
| TMP269 | 1314890-29-3 | free base | HDAC | 86.1 | -0.01 | 117.9 | 1.16 | 73.2 | -1.07 | 77.0 | -0.50 |
| Tofacitinib (CP-690550) Citrate | 540737-29-9 | citrate | JAK | 86.8 | 0.02 | 97.1 | 0.40 | 75.7 | -0.97 | 123.7 | 0.98 |
| Tofacitinib (CP-690550,Tasocitinib) | 477600-75-2 | free base | JAK | 95.3 | 0.38 | 81.8 | -0.15 | 94.3 | -0.18 | 109.4 | 0.52 |
| Tolazoline HCl | 59-97-2 | free base | Adrenergic Receptor | 83.8 | -0.11 | 117.7 | 1.15 | 76.4 | -0.94 | 117.2 | 0.77 |
| Tolbutamide | 64-77-7 | free base | Potassium Channel | 121.1 | 1.47 | 67.2 | -0.68 | 91.3 | -0.30 | 118.6 | 0.82 |
| Tolcapone | 134308-13-7 | free base | Transferase | 88.5 | 0.09 | 117.8 | 1.16 | 101.0 | 0.11 | 120.6 | 0.88 |
| Tolfenamic Acid | 13710-19-5 | free base | COX | 89.9 | 0.15 | 68.1 | -0.65 | 103.6 | 0.22 | 91.7 | -0.03 |
| Tolterodine tartrate | 124937-52-6 | tartrate | AChR | 100.2 | 0.58 | 115.4 | 1.07 | 125.1 | 1.13 | 138.4 | 1.44 |
| Tolvaptan | 150683-30-0 | free base | Vasopressin Receptor | 78.9 | -0.32 | 116.7 | 1.12 | 112.5 | 0.60 | 121.3 | 0.90 |
| Topiramate | 97240-79-4 | free base | Carbonic Anhydrase | 102.5 | 0.68 | 72.7 | -0.48 | 107.1 | 0.37 | 71.8 | -0.67 |
| Topotecan HCl | 119413-54-6 | hydrochloride | Topoisomerase | 47.1 | -1.66 | 54.4 | -1.15 | 95.5 | -0.13 | 7.9 | -2.69 |
| Torcetrapib | 262352-17-0 | free base | CETP | 98.9 | 0.53 | 90.0 | 0.15 | 98.7 | 0.01 | 101.9 | 0.29 |
| Toremifene Citrate | 89778-27-8 | citrate | Estrogen/progestogen Receptor | 125.7 | 1.66 | 98.1 | 0.44 | 121.2 | 0.97 | 104.1 | 0.36 |
| Torin 2 | 1223001-51-1 | free base | ATM/ATR,mTOR | 40.2 | -1.96 | 35.1 | -1.85 | 57.7 | -1.73 | 8.8 | -2.66 |
| TPCA-1 | 507475-17-4 | free base | IκB/IKK | 71.0 | -0.65 | 114.5 | 1.04 | 119.5 | 0.89 | 96.2 | 0.11 |
| Trametinib (GSK1120212) | 871700-17-3 | free base | MEK | 72.1 | -0.61 | 36.4 | -1.80 | 60.2 | -1.63 | 106.9 | 0.45 |
| Tranylcypromine (2-PCPA) HCl | 4548-34-9 | hydrochloride | Histone demethylases | 80.9 | -0.23 | 62.7 | -0.85 | 79.8 | -0.79 | 100.3 | 0.24 |
| Trelagliptin | 865759-25-7 | free base | DDP-4 | 83.8 | -0.11 | 67.1 | -0.69 | 79.2 | -0.82 | 114.1 | 0.68 |
| Triamterene | 396-01-0 | free base | Sodium Channel | 93.2 | 0.29 | 102.8 | 0.61 | 99.5 | 0.04 | 109.5 | 0.53 |
| Triapine | 200933-27-3 | free base | ribonucleotide reductase | 78.3 | -0.34 | 116.3 | 1.10 | 89.8 | -0.37 | 25.7 | -2.12 |
| Trichostatin A (TSA) | 58880-19-6 | free base | HDAC | 52.2 | -1.45 | 47.0 | -1.42 | 38.2 | -2.56 | 2.0 | -2.88 |
| Triciribine | 35943-35-2 | free base | Akt | 79.8 | -0.28 | 116.5 | 1.11 | 118.7 | 0.86 | 52.8 | -1.27 |

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|--|--------------|---------------|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Trifluoperazine 2HCl | 440-17-5 | 2HCl | Autophagy | 96.9 | 0.45 | 117.4 | 1.14 | 132.5 | 1.44 | 135.3 | 1.35 |
| Triflusal | 322-79-2 | free base | COX | 91.6 | 0.22 | 118.0 | 1.16 | 93.7 | -0.20 | 130.1 | 1.18 |
| Trilostane | 13647-35-3 | free base | Dehydrogenase | 78.0 | -0.36 | 115.9 | 1.09 | 102.9 | 0.19 | 89.7 | -0.10 |
| Trimebutine | 39133-31-8 | free base | Opioid Receptor | 101.8 | 0.65 | 115.3 | 1.06 | 95.2 | -0.14 | 126.2 | 1.06 |
| Tripelennamine HCl | 154-69-8 | hydrochloride | Histamine Receptor | 87.3 | 0.04 | 118.3 | 1.17 | 115.0 | 0.70 | 108.0 | 0.48 |
| Tropicamide | 1508-75-4 | free base | AChR | 94.7 | 0.35 | 116.3 | 1.10 | 109.4 | 0.46 | 156.7 | 2.02 |
| Tropisetron | 105826-92-4 | hydrochloride | 5-HT Receptor | 101.1 | 0.62 | 117.0 | 1.13 | 106.8 | 0.35 | 90.4 | -0.08 |
| Trospium chloride | 10405-02-4 | chloride | AChR | 80.1 | -0.27 | 96.8 | 0.39 | 122.0 | 1.00 | 92.9 | 0.00 |
| TSU-68 (SU6668, Orantinib) | 252916-29-3 | free base | VEGFR,PDGFR,FGFR | 100.6 | 0.60 | 67.0 | -0.69 | 127.8 | 1.25 | 72.3 | -0.65 |
| Tubacin | 537049-40-4 | free base | HDAC | 106.3 | 0.84 | 54.6 | -1.14 | 77.6 | -0.89 | 97.6 | 0.15 |
| Tubastatin A | 1252003-15-8 | free base | HDAC | 62.3 | -1.02 | 61.7 | -0.88 | 111.1 | 0.54 | 81.4 | -0.36 |
| Tubastatin A HCl | 1310693-92-5 | hydrochloride | HDAC | 71.4 | -0.64 | 115.7 | 1.08 | 107.6 | 0.39 | 103.3 | 0.33 |
| TW-37 | 877877-35-5 | free base | Bcl-2 | 103.5 | 0.72 | 106.1 | 0.73 | 109.2 | 0.46 | 85.6 | -0.23 |
| TWS119 | 601514-19-6 | free base | GSK-3 | 102.4 | 0.68 | 115.6 | 1.08 | 101.7 | 0.14 | 83.3 | -0.30 |
| Tyrphostin 9 | 10537-47-0 | free base | EGFR | 49.9 | -1.55 | 49.4 | -1.33 | 109.2 | 0.46 | 93.4 | 0.02 |
| Tyrphostin AG 1296 | 146535-11-7 | free base | FGFR,c-Kit,PDGFR | 88.9 | 0.11 | 70.8 | -0.55 | 81.1 | -0.74 | 96.2 | 0.11 |
| Tyrphostin AG 879 | 148741-30-4 | free base | HER2 | 73.5 | -0.55 | 68.8 | -0.63 | 102.3 | 0.16 | 109.2 | 0.52 |
| U0126-EtOH | 1173097-76-1 | ethanolat | MEK | 86.6 | 0.01 | 66.6 | -0.71 | 73.5 | -1.06 | 77.6 | -0.48 |
| U-104 | 178606-66-1 | free base | Carbonic Anhydrase | 84.3 | -0.09 | 46.1 | -1.45 | 102.9 | 0.19 | 100.8 | 0.25 |
| UK 383367 | 348622-88-8 | free base | Procollagen C Proteinase | 104.4 | 0.76 | 88.9 | 0.11 | 90.5 | -0.34 | 135.8 | 1.36 |
| UNC1215 | 1415800-43-9 | free base | Epigenetic Reader Domain | 97.6 | 0.47 | 80.1 | -0.21 | | | 98.3 | 0.17 |
| UNC1999 | 1431612-23-5 | free base | Histone Methyltransferase | 77.9 | -0.36 | 70.8 | -0.55 | | | 111.4 | 0.59 |
| UNC2881 | 1493764-08-1 | free base | Others | 75.9 | -0.44 | 117.5 | 1.14 | 88.3 | -0.43 | 79.4 | -0.43 |
| UNC669 | 1314241-44-5 | free base | MBT | 73.5 | -0.55 | 116.8 | 1.12 | 96.4 | -0.09 | 109.8 | 0.54 |
| UPF 1069 | 1048371-03-4 | free base | PARP | 65.2 | -0.90 | 85.7 | -0.01 | 82.9 | -0.66 | 76.5 | -0.52 |
| Urapidil HCl | 64887-14-5 | hydrochloride | 5-HT Receptor | 106.3 | 0.84 | 67.3 | -0.68 | 100.2 | 0.07 | 146.7 | 1.71 |
| URB597 | 546141-08-6 | free base | FAAH | 89.7 | 0.14 | 105.5 | 0.71 | 127.7 | 1.24 | 128.7 | 1.14 |
| Valdecoxib | 181695-72-7 | free base | COX | 101.2 | 0.63 | 114.7 | 1.04 | 104.6 | 0.26 | 120.9 | 0.89 |
| Valproic acid sodium salt (Sodium | 1069-66-5 | free base | Autophagy,HDAC,GABA | 79.8 | -0.28 | 92.4 | 0.23 | 112.7 | 0.61 | 82.2 | -0.33 |

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| valproate) | | | Receptor | | | | | | | | | |
| Valsartan | 137862-53-4 | free base | RAAS | 101.2 | 0.63 | 116.8 | 1.12 | 101.7 | 0.14 | 83.8 | -0.28 | |
| Vandetanib (ZD6474) | 443913-73-3 | free base | VEGFR | 104.1 | 0.75 | 104.4 | 0.67 | 90.2 | -0.35 | 111.9 | 0.61 | |
| Vardenafil HCl Trihydrate | 224785-90-4 | hydrate | PDE | 97.4 | 0.47 | 51.8 | -1.24 | 117.1 | 0.79 | 143.1 | 1.59 | |
| Varespladib (LY315920) | 172732-68-2 | free base | Phospholipase (e.g. PLA) | 86.5 | 0.00 | 109.7 | 0.86 | 99.1 | 0.03 | 109.2 | 0.52 | |
| Varlitinib | 845272-21-1 | free base | EGFR | 76.1 | -0.44 | 113.5 | 1.00 | 112.9 | 0.61 | 151.7 | 1.87 | |
| Vatalanib (PTK787) 2HCl | 212141-51-0 | dihydrochloride | c-Kit,VEGFR | 90.5 | 0.17 | 100.9 | 0.54 | 99.6 | 0.05 | 108.1 | 0.48 | |
| WAY-100635 Maleate | 1092679-51-0 | hydrochloride | 5-HT Receptor | 107.0 | 0.87 | 114.6 | 1.04 | 116.3 | 0.76 | 107.5 | 0.47 | |
| WAY-600 | 1062159-35-6 | free base | mTOR | 57.3 | -1.23 | 113.5 | 1.00 | 91.0 | -0.32 | 98.8 | 0.19 | |
| VE-821 | 1232410-49-9 | free base | ATM/ATR | 83.0 | -0.15 | 56.8 | -1.06 | 104.9 | 0.27 | 100.4 | 0.24 | |
| VE-822 | 1232416-25-9 | free base | ATM/ATR | 83.8 | -0.11 | 45.3 | -1.48 | | | 33.8 | -1.87 | |
| Veliparib (ABT-888) | 912444-00-9 | free base | PARP | 114.6 | 1.19 | 106.7 | 0.75 | 93.3 | -0.22 | 51.0 | -1.32 | |
| Vemurafenib (PLX4032, RG7204) | 918504-65-1 | free base | Raf | 110.9 | 1.04 | 66.2 | -0.72 | 184.8 | 3.67 | 86.8 | -0.19 | |
| Venlafaxine | 99300-78-4 | hydrochloride | 5-HT Receptor | 76.3 | -0.43 | 92.2 | 0.22 | 106.8 | 0.35 | 99.1 | 0.20 | |
| VER-49009 | 940289-57-6 | free base | HSP90 | 48.1 | -1.62 | 89.2 | 0.12 | 57.1 | -1.76 | 73.4 | -0.61 | |
| VER-50589 | 747413-08-7 | free base | HSP (e.g. HSP90) | 49.5 | -1.57 | 36.3 | -1.81 | 40.0 | -2.48 | 50.7 | -1.33 | |
| WH-4-023 | 837422-57-8 | free base | Src | 95.1 | 0.37 | 66.9 | -0.70 | 109.5 | 0.47 | 111.2 | 0.58 | |
| WHI-P154 | 211555-04-3 | free base | JAK,EGFR | 80.7 | -0.24 | 114.4 | 1.03 | 105.8 | 0.31 | 105.6 | 0.40 | |
| WIKI4 | 838818-26-1 | free base | Wnt/beta-catenin | 119.1 | 1.38 | 107.1 | 0.77 | 98.3 | -0.01 | 89.8 | -0.09 | |
| Vildagliptin (LAF-237) | 274901-16-5 | free base | DPP-4 | 103.5 | 0.72 | 119.3 | 1.21 | 112.9 | 0.61 | 125.5 | 1.04 | |
| Vinorelbine Tartrate | 125317-39-7 | Salt | Microtubule Associat | 49.9 | -1.55 | 51.4 | -1.26 | 48.7 | -2.11 | 23.9 | -2.18 | |
| Vismodegib (GDC-0449) | 879085-55-9 | free base | Hedgehog/Smoothened | 91.8 | 0.23 | 86.1 | 0.00 | 103.5 | 0.21 | 107.0 | 0.45 | |
| Wnt-C59 (C59) | 1243243-89-1 | free base | Wnt/beta-catenin | 85.4 | -0.04 | 73.5 | -0.46 | 88.5 | -0.42 | 117.3 | 0.78 | |
| Wnt-C59 (C59) | 1243243-89-1 | free base | Wnt/beta-catenin | 92.7 | 0.26 | 62.6 | -0.85 | 81.6 | -0.72 | 119.7 | 0.85 | |
| Volasertib (BI 6727) | 755038-65-4 | free base | PLK | 54.5 | -1.35 | 43.5 | -1.55 | 33.8 | -2.75 | 6.1 | -2.75 | |
| Voreloxin (SNS-595) | 175414-77-4 | free base | Topoisomerase | 52.5 | -1.44 | 71.9 | -0.51 | 96.7 | -0.07 | 66.5 | -0.83 | |
| Voriconazole | 137234-62-9 | free base | P450 (e.g. CYP17) | 71.6 | -0.63 | 113.0 | 0.98 | 100.5 | 0.08 | 93.5 | 0.02 | |
| Vorinostat (SAHA, MK0683) | 149647-78-9 | free base | Autophagy,HDAC | 71.2 | -0.64 | 68.1 | -0.65 | 92.3 | -0.26 | 14.5 | -2.48 | |

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| Vortioxetine (Lu AA21004) HBr | 960203-27-4 | hydrobromide | 5-HT Receptor | 76.3 | -0.43 | 62.3 | -0.86 | 102.4 | 0.17 | 138.8 | 1.46 |
| Wortmannin | 19545-26-7 | free base | Autophagy,ATM/ATR,PI3K | 85.4 | -0.04 | 107.7 | 0.79 | 127.8 | 1.25 | 123.1 | 0.96 |
| WP1066 | 857064-38-1 | free base | JAK | 96.0 | 0.41 | 102.5 | 0.60 | 101.5 | 0.13 | 102.1 | 0.30 |
| VS-5584 (SB2343) | 1246560-33-7 | free base | PI3K | 35.0 | -2.18 | 43.7 | -1.54 | 45.5 | -2.25 | 48.2 | -1.41 |
| VU 0357121 | 433967-28-3 | free base | GluR | 96.5 | 0.43 | 91.4 | 0.19 | 103.5 | 0.22 | 107.8 | 0.48 |
| VU 0361737 | 1161205-04-4 | free base | GluR | 108.4 | 0.93 | 114.5 | 1.04 | 109.5 | 0.47 | 105.9 | 0.41 |
| VU 0364439 | 1246086-78-1 | free base | GluR | 101.9 | 0.66 | 63.9 | -0.80 | 103.4 | 0.21 | 115.9 | 0.73 |
| VU 0364770 | 61350-00-3 | free base | GluR | 83.8 | -0.11 | 113.5 | 1.00 | 124.5 | 1.11 | 113.4 | 0.65 |
| VUF 10166 | 155584-74-0 | free base | 5-HT Receptor | 88.6 | 0.09 | 114.4 | 1.03 | 107.2 | 0.37 | 113.0 | 0.64 |
| VX-222 (VCH-222, Lomibuvir) | 1026785-59-0 | free base | HCV Protease | 101.2 | 0.63 | 110.5 | 0.89 | 110.6 | 0.51 | 86.9 | -0.19 |
| VX-661 | 1152311-62-0 | free base | CFTR | 79.1 | -0.31 | 74.5 | -0.42 | 105.6 | 0.30 | 107.1 | 0.45 |
| VX-680 (Tozasertib, MK-0457) | 639089-54-6 | free base | Aurora Kinase | 62.0 | -1.03 | 62.2 | -0.87 | 46.2 | -2.22 | 76.1 | -0.53 |
| VX-702 | 745833-23-2 | free base | p38 MAPK | 91.8 | 0.23 | 56.2 | -1.08 | 81.0 | -0.74 | 88.8 | -0.13 |
| VX-745 | 209410-46-8 | free base | p38 MAPK | 72.7 | -0.58 | 112.3 | 0.95 | 95.3 | -0.14 | 83.9 | -0.28 |
| VX-765 | 273404-37-8,851091-96-8 | free base | Caspase | 104.7 | 0.78 | 54.7 | -1.14 | 93.3 | -0.22 | 91.0 | -0.06 |
| VX-809 (Lumacaftor) | 936727-05-8 | free base | CFTR | 116.1 | 1.26 | 101.5 | 0.56 | 111.8 | 0.57 | 77.1 | -0.50 |
| WY-14643 (Pirinixic Acid) | 50892-23-4 | free base | PPAR | 81.9 | -0.19 | 63.8 | -0.81 | 104.3 | 0.25 | 129.9 | 1.18 |
| WYE-125132 (WYE-132) | 1144068-46-1 | free base | mTOR | 56.2 | -1.28 | 70.6 | -0.56 | 41.7 | -2.41 | 39.9 | -1.68 |
| WYE-354 | 1062169-56-5 | free base | mTOR | 92.2 | 0.25 | 112.3 | 0.96 | 98.8 | 0.01 | 74.3 | -0.59 |
| WZ3146 | 1214265-56-1 | free base | EGFR | 102.5 | 0.68 | 89.2 | 0.12 | 91.7 | -0.29 | 60.6 | -1.02 |
| WZ4002 | 1213269-23-8 | free base | EGFR | 117.3 | 1.31 | 79.2 | -0.25 | 107.6 | 0.39 | 95.8 | 0.09 |
| WZ4003 | 1214265-58-3 | free base | AMPK | 123.7 | 1.58 | 78.5 | -0.27 | 104.4 | 0.25 | 100.1 | 0.23 |
| WZ8040 | 1214265-57-2 | free base | EGFR | 97.1 | 0.45 | 75.5 | -0.38 | 122.9 | 1.04 | 79.1 | -0.44 |
| WZ811 | 55778-02-4 | free base | CXCR | 75.3 | -0.47 | 58.5 | -1.00 | 101.8 | 0.14 | 108.6 | 0.50 |
| XAV-939 | 284028-89-3 | free base | Wnt/beta-catenin | 93.5 | 0.30 | 69.2 | -0.61 | 107.8 | 0.40 | 91.3 | -0.05 |
| XL019 | 945755-56-6 | free base | JAK | 76.0 | -0.44 | 112.4 | 0.96 | 87.9 | -0.45 | 110.9 | 0.57 |
| XL019 | 945755-56-6 | free base | JAK | 68.7 | -0.75 | 60.9 | -0.91 | 86.6 | -0.50 | 118.6 | 0.82 |
| XL147 | 956958-53-5 | free base | PI3K | 116.1 | 1.26 | 115.1 | 1.06 | 108.0 | 0.40 | 85.0 | -0.25 |

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| XL335 | 629664-81-9 | free base | FXR | 85.2 | -0.05 | 114.6 | 1.04 | 114.9 | 0.70 | 107.3 | 0.46 |
| XL888 | 1149705-71-4 | free base | HSP (e.g. HSP90) | 45.1 | -1.75 | 30.8 | -2.01 | | | 40.1 | -1.67 |
| XMD8-92 | 1234480-50-2 | free base | ERK | 68.8 | -0.75 | 75.8 | -0.37 | 94.4 | -0.17 | 73.3 | -0.62 |
| Xylazine HCl | 23076-35-9 | hydrochloride | Adrenergic Receptor | 91.8 | 0.23 | 115.5 | 1.07 | 144.9 | 1.97 | 131.2 | 1.22 |
| Y-27632 2HCl | 129830-38-2 | dihydrochloric | Autophagy,ROCK | 112.7 | 1.11 | 107.7 | 0.79 | 74.4 | -1.02 | 118.9 | 0.83 |
| YH239-EE | 1364488-67-4 | free base | Mdm2 | 126.0 | 1.68 | 107.4 | 0.78 | 108.8 | 0.44 | 84.7 | -0.26 |
| YM155 (Sepantronium Bromide) | 781661-94-7 | bromide | Survivin | 35.2 | -2.17 | 1.9 | -3.06 | 2.1 | -4.09 | 0.4 | -2.93 |
| YM201636 | 371942-69-7 | free base | PI3K | 89.9 | 0.15 | 90.5 | 0.16 | 95.6 | -0.12 | 74.5 | -0.58 |
| YO-01027 | 209984-56-5 | free base | Gamma-secretase | 87.8 | 0.06 | 55.8 | -1.10 | 138.9 | 1.72 | 116.9 | 0.76 |
| Zalcitabine | 7481-89-2 | free base | Reverse Transcriptase | 125.8 | 1.67 | 109.4 | 0.85 | 97.5 | -0.04 | 95.3 | 0.08 |
| Zaltoprofen | 74711-43-6 | free base | COX | 130.8 | 1.88 | 115.4 | 1.07 | 112.6 | 0.60 | 121.9 | 0.92 |
| ZCL278 | 587841-73-4 | free base | Rac | 91.4 | 0.21 | 116.7 | 1.12 | 109.5 | 0.47 | 107.8 | 0.47 |
| Zebularine | 3690-10-6 | free base | DNA Methyltransferase | 70.3 | -0.68 | 52.3 | -1.22 | | | 94.1 | 0.04 |
| Z-FA-FMK | 197855-65-5 | free base | Cysteine Protease | 136.5 | 2.12 | 106.8 | 0.76 | 115.0 | 0.70 | 106.5 | 0.43 |
| Zibotentan (ZD4054) | 186497-07-4 | free base | Endothelin Receptor | 105.0 | 0.79 | 112.8 | 0.97 | 108.9 | 0.44 | 67.1 | -0.81 |
| Zidovudine | 30516-87-1 | free base | Reverse Transcriptase | 109.8 | 0.99 | 116.3 | 1.10 | 114.4 | 0.68 | 94.5 | 0.05 |
| Zinc Pyrithione | 13463-41-7 | free base | Proton Pump | 118.8 | 1.37 | 109.4 | 0.85 | 109.8 | 0.48 | 62.1 | -0.97 |
| ZM 306416 | 690206-97-4 | free base | VEGFR | 81.1 | -0.22 | 114.8 | 1.05 | 98.0 | -0.02 | 115.4 | 0.72 |
| ZM 323881 HCl | 193000-39-4 | hydrochloride | VEGFR | 96.0 | 0.41 | 114.0 | 1.02 | 95.5 | -0.12 | 94.6 | 0.06 |
| ZM 336372 | 208260-29-1 | free base | Raf | 72.6 | -0.58 | 74.2 | -0.43 | 111.2 | 0.54 | 128.3 | 1.13 |
| ZM 39923 HCl | 1021868-92-7 | hydrochloride | JAK | 60.3 | -1.11 | 61.8 | -0.88 | 92.9 | -0.24 | 79.1 | -0.44 |
| ZM 447439 | 331771-20-1 | free base | Aurora Kinase | 100.5 | 0.60 | 77.3 | -0.32 | 74.5 | -1.02 | 93.8 | 0.03 |
| Zolmitriptan | 139264-17-8 | free base | 5-HT Receptor | 87.6 | 0.05 | 115.2 | 1.06 | 97.6 | -0.03 | 94.4 | 0.05 |
| Zosuquidar (LY335979) 3HCl | 167465-36-3 | hydrochloride | P-gp | 84.7 | -0.07 | 112.2 | 0.95 | 125.6 | 1.15 | 90.4 | -0.08 |
| Zotarolimus(ABT-578) | 221877-54-9 | free base | mTOR | 63.7 | -0.96 | 81.6 | -0.16 | | | 71.5 | -0.68 |
| ZSTK474 | 475110-96-4 | free base | PI3K | 51.6 | -1.48 | 94.9 | 0.32 | 63.0 | -1.51 | 90.4 | -0.08 |
| Z-VAD-FMK | 187389-52-2 | free base | Caspase | 92.5 | 0.26 | 66.1 | -0.72 | 79.1 | -0.82 | 99.9 | 0.22 |